Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 09:33 pm BST

PDB ID	:	5JJ1
Title	:	Structure of the Immature Procapsid Conformation of P22 Portal Protein
Authors	:	Lokareddy, R.K.; Cingolani, G.
Deposited on	:	2016-04-22
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

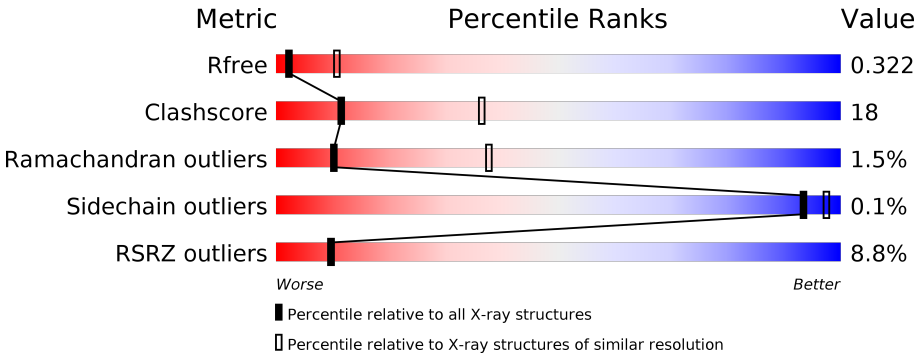
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	610	7% 62% 33%
1	B	610	6% 59% 35%
1	C	610	9% 57% 38%
1	D	610	10% 58% 35%
1	E	610	8% 60% 34%
1	F	610	7% 59% 36%

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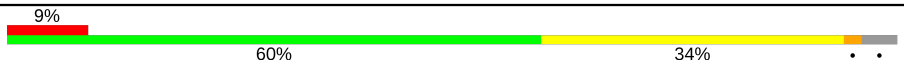
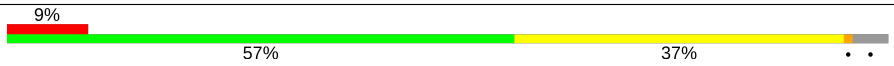
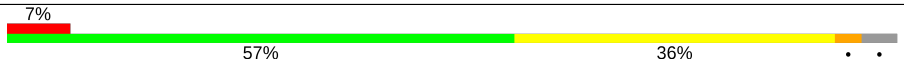
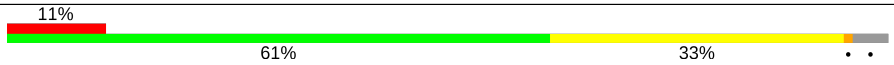
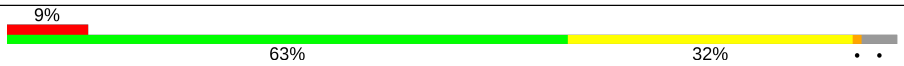
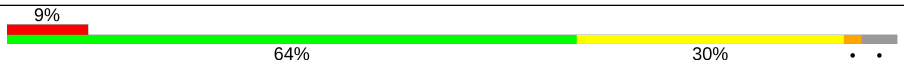
Mol	Chain	Length	Quality of chain
1	G	610	
1	H	610	
1	I	610	
1	J	610	
1	K	610	
1	L	610	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 56559 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4724	2976	806	921	21			
1	B	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	C	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	D	585	Total	C	N	O	S	0	0	0
			4723	2977	805	920	21			
1	E	585	Total	C	N	O	S	0	0	0
			4720	2974	805	920	21			
1	F	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	G	585	Total	C	N	O	S	0	0	0
			4706	2966	804	915	21			
1	H	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	I	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	J	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			
1	K	585	Total	C	N	O	S	0	0	0
			4716	2971	805	919	21			
1	L	585	Total	C	N	O	S	0	0	0
			4710	2968	804	917	21			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	LEU	-	expression tag	UNP P26744
A	604	GLU	-	expression tag	UNP P26744
A	605	HIS	-	expression tag	UNP P26744
A	606	HIS	-	expression tag	UNP P26744
A	607	HIS	-	expression tag	UNP P26744

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP P26744
A	609	HIS	-	expression tag	UNP P26744
A	610	HIS	-	expression tag	UNP P26744
B	603	LEU	-	expression tag	UNP P26744
B	604	GLU	-	expression tag	UNP P26744
B	605	HIS	-	expression tag	UNP P26744
B	606	HIS	-	expression tag	UNP P26744
B	607	HIS	-	expression tag	UNP P26744
B	608	HIS	-	expression tag	UNP P26744
B	609	HIS	-	expression tag	UNP P26744
B	610	HIS	-	expression tag	UNP P26744
C	603	LEU	-	expression tag	UNP P26744
C	604	GLU	-	expression tag	UNP P26744
C	605	HIS	-	expression tag	UNP P26744
C	606	HIS	-	expression tag	UNP P26744
C	607	HIS	-	expression tag	UNP P26744
C	608	HIS	-	expression tag	UNP P26744
C	609	HIS	-	expression tag	UNP P26744
C	610	HIS	-	expression tag	UNP P26744
D	603	LEU	-	expression tag	UNP P26744
D	604	GLU	-	expression tag	UNP P26744
D	605	HIS	-	expression tag	UNP P26744
D	606	HIS	-	expression tag	UNP P26744
D	607	HIS	-	expression tag	UNP P26744
D	608	HIS	-	expression tag	UNP P26744
D	609	HIS	-	expression tag	UNP P26744
D	610	HIS	-	expression tag	UNP P26744
E	603	LEU	-	expression tag	UNP P26744
E	604	GLU	-	expression tag	UNP P26744
E	605	HIS	-	expression tag	UNP P26744
E	606	HIS	-	expression tag	UNP P26744
E	607	HIS	-	expression tag	UNP P26744
E	608	HIS	-	expression tag	UNP P26744
E	609	HIS	-	expression tag	UNP P26744
E	610	HIS	-	expression tag	UNP P26744
F	603	LEU	-	expression tag	UNP P26744
F	604	GLU	-	expression tag	UNP P26744
F	605	HIS	-	expression tag	UNP P26744
F	606	HIS	-	expression tag	UNP P26744
F	607	HIS	-	expression tag	UNP P26744
F	608	HIS	-	expression tag	UNP P26744
F	609	HIS	-	expression tag	UNP P26744

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Chain	Residue	Modelled	Actual	Comment	Reference
F	610	HIS	-	expression tag	UNP P26744
G	603	LEU	-	expression tag	UNP P26744
G	604	GLU	-	expression tag	UNP P26744
G	605	HIS	-	expression tag	UNP P26744
G	606	HIS	-	expression tag	UNP P26744
G	607	HIS	-	expression tag	UNP P26744
G	608	HIS	-	expression tag	UNP P26744
G	609	HIS	-	expression tag	UNP P26744
G	610	HIS	-	expression tag	UNP P26744
H	603	LEU	-	expression tag	UNP P26744
H	604	GLU	-	expression tag	UNP P26744
H	605	HIS	-	expression tag	UNP P26744
H	606	HIS	-	expression tag	UNP P26744
H	607	HIS	-	expression tag	UNP P26744
H	608	HIS	-	expression tag	UNP P26744
H	609	HIS	-	expression tag	UNP P26744
H	610	HIS	-	expression tag	UNP P26744
I	603	LEU	-	expression tag	UNP P26744
I	604	GLU	-	expression tag	UNP P26744
I	605	HIS	-	expression tag	UNP P26744
I	606	HIS	-	expression tag	UNP P26744
I	607	HIS	-	expression tag	UNP P26744
I	608	HIS	-	expression tag	UNP P26744
I	609	HIS	-	expression tag	UNP P26744
I	610	HIS	-	expression tag	UNP P26744
J	603	LEU	-	expression tag	UNP P26744
J	604	GLU	-	expression tag	UNP P26744
J	605	HIS	-	expression tag	UNP P26744
J	606	HIS	-	expression tag	UNP P26744
J	607	HIS	-	expression tag	UNP P26744
J	608	HIS	-	expression tag	UNP P26744
J	609	HIS	-	expression tag	UNP P26744
J	610	HIS	-	expression tag	UNP P26744
K	603	LEU	-	expression tag	UNP P26744
K	604	GLU	-	expression tag	UNP P26744
K	605	HIS	-	expression tag	UNP P26744
K	606	HIS	-	expression tag	UNP P26744
K	607	HIS	-	expression tag	UNP P26744
K	608	HIS	-	expression tag	UNP P26744
K	609	HIS	-	expression tag	UNP P26744
K	610	HIS	-	expression tag	UNP P26744
L	603	LEU	-	expression tag	UNP P26744

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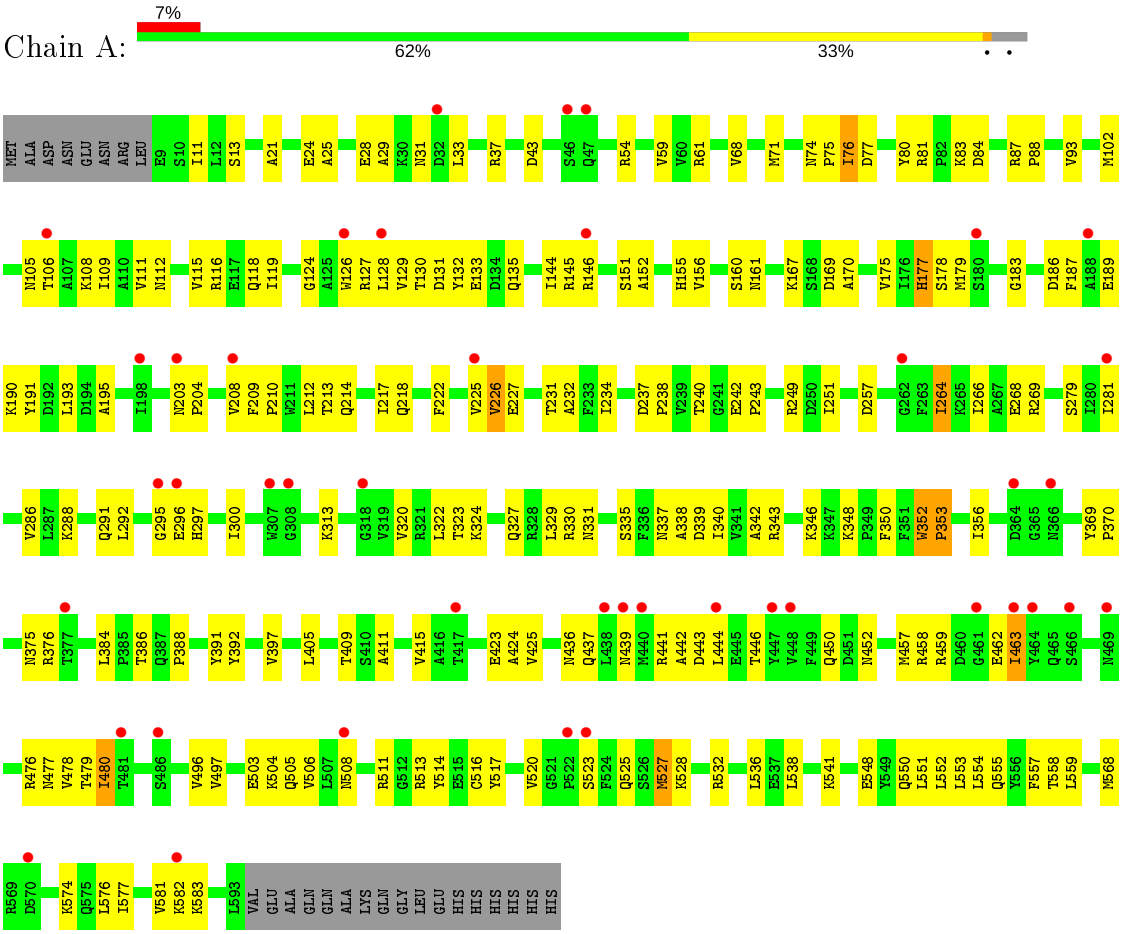
Chain	Residue	Modelled	Actual	Comment	Reference
L	604	GLU	-	expression tag	UNP P26744
L	605	HIS	-	expression tag	UNP P26744
L	606	HIS	-	expression tag	UNP P26744
L	607	HIS	-	expression tag	UNP P26744
L	608	HIS	-	expression tag	UNP P26744
L	609	HIS	-	expression tag	UNP P26744
L	610	HIS	-	expression tag	UNP P26744

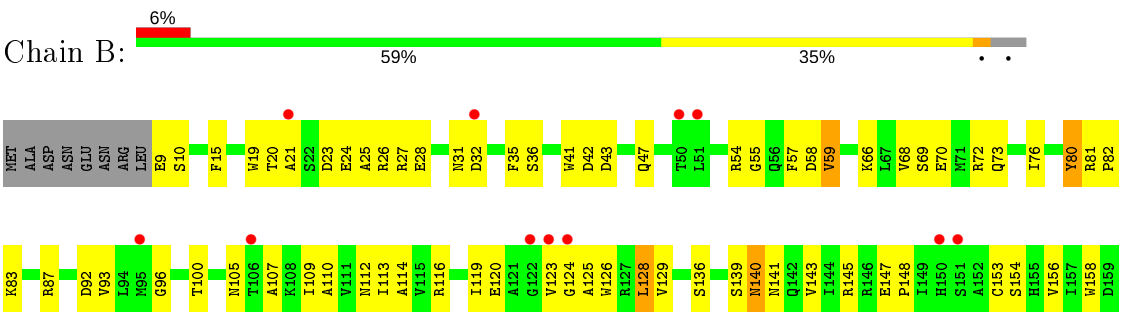
3 Residue-property plots (i)

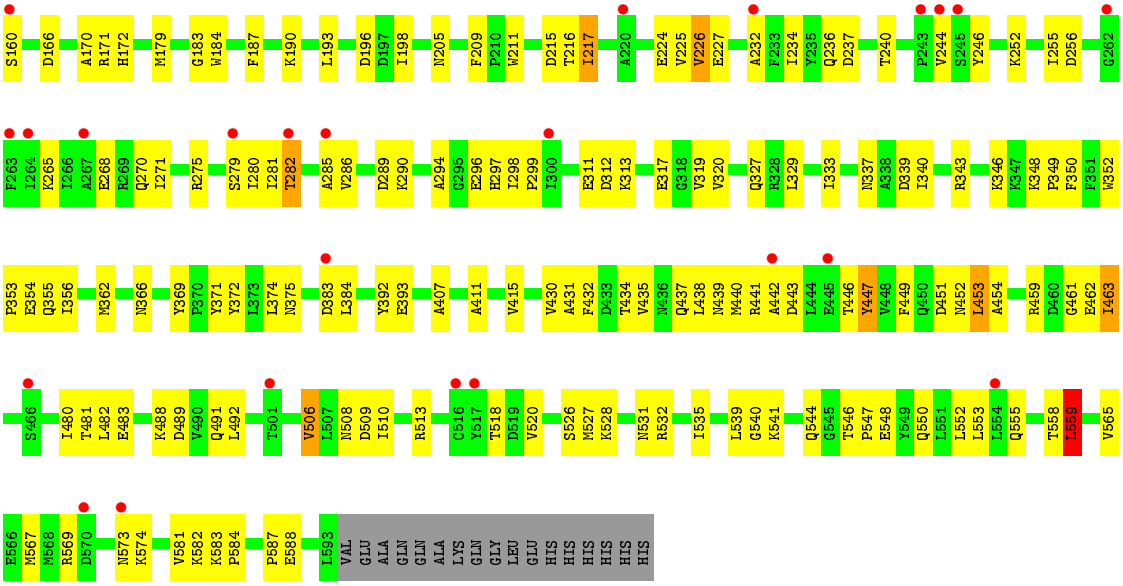
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Portal protein



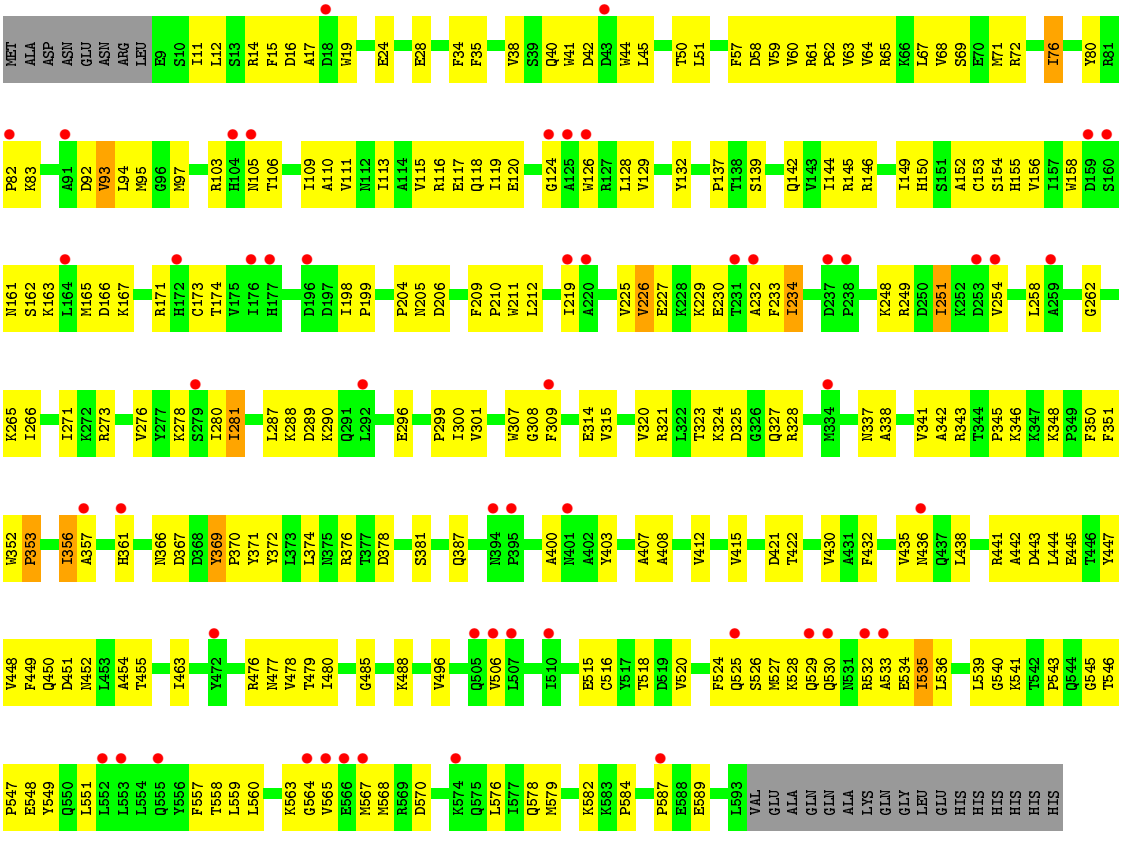
- Molecule 1: Portal protein





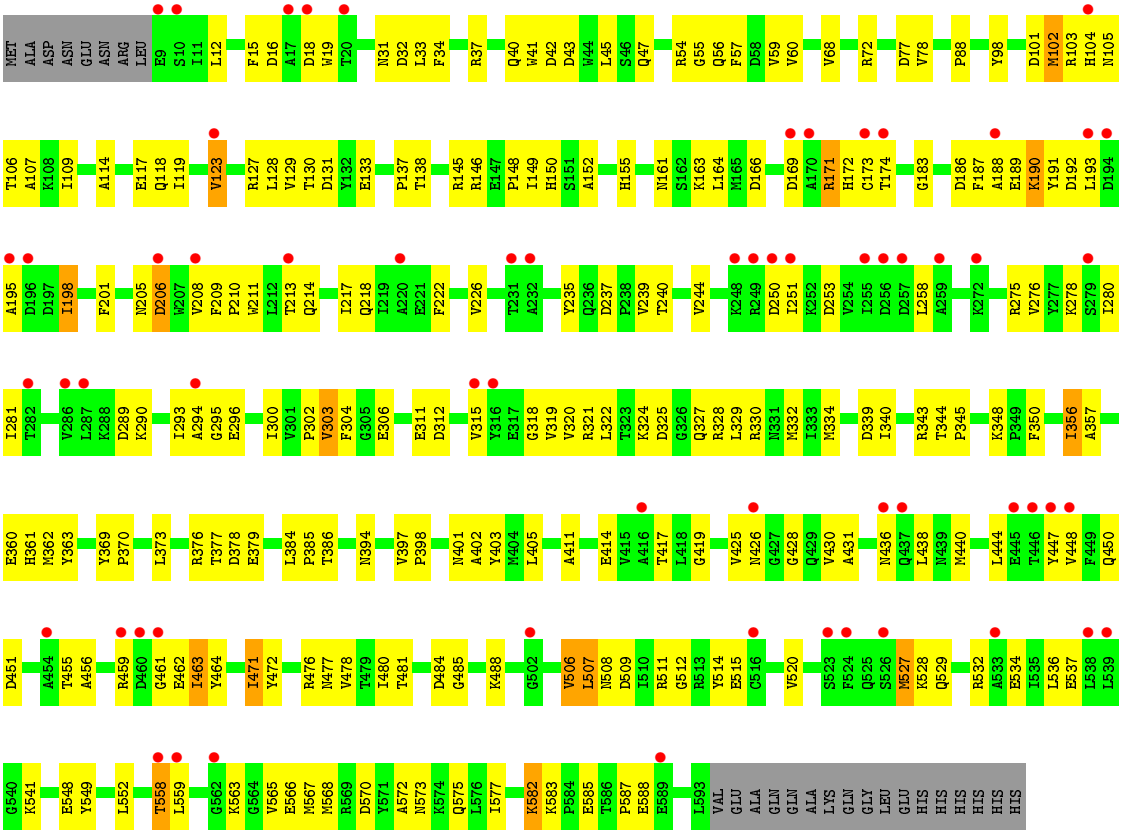
- Molecule 1: Portal protein

Chain C:



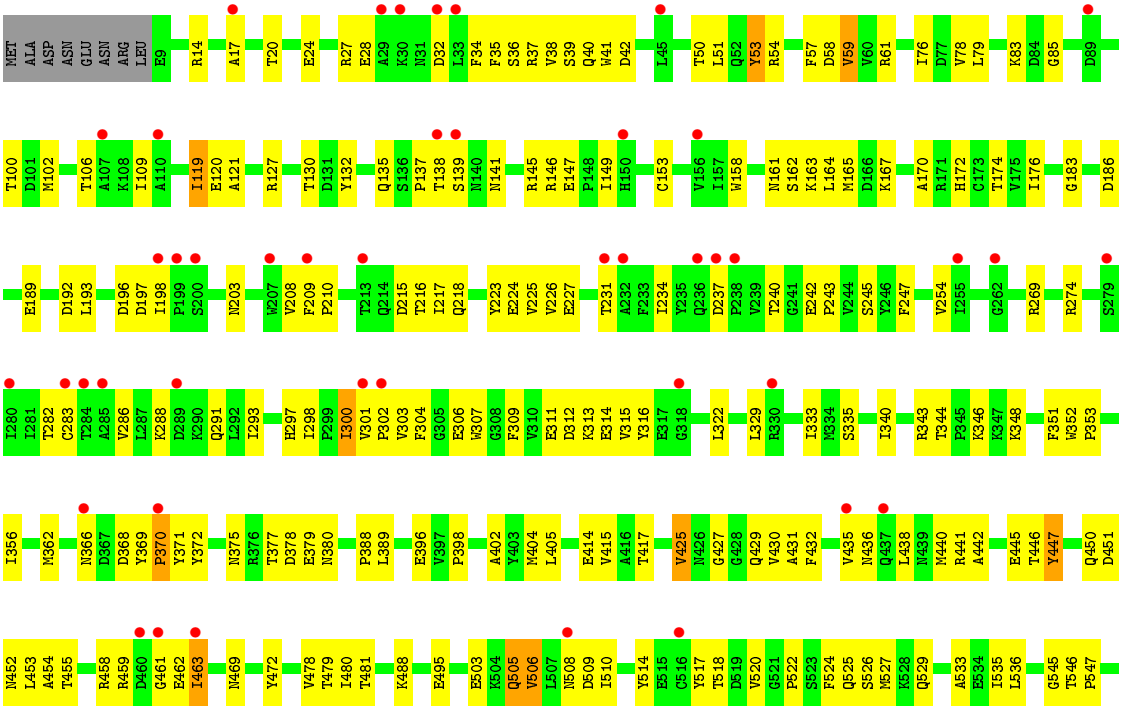
- Molecule 1: Portal protein

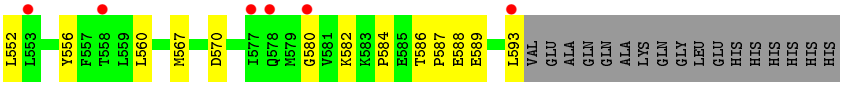
Chain D:



• Molecule 1: Portal protein

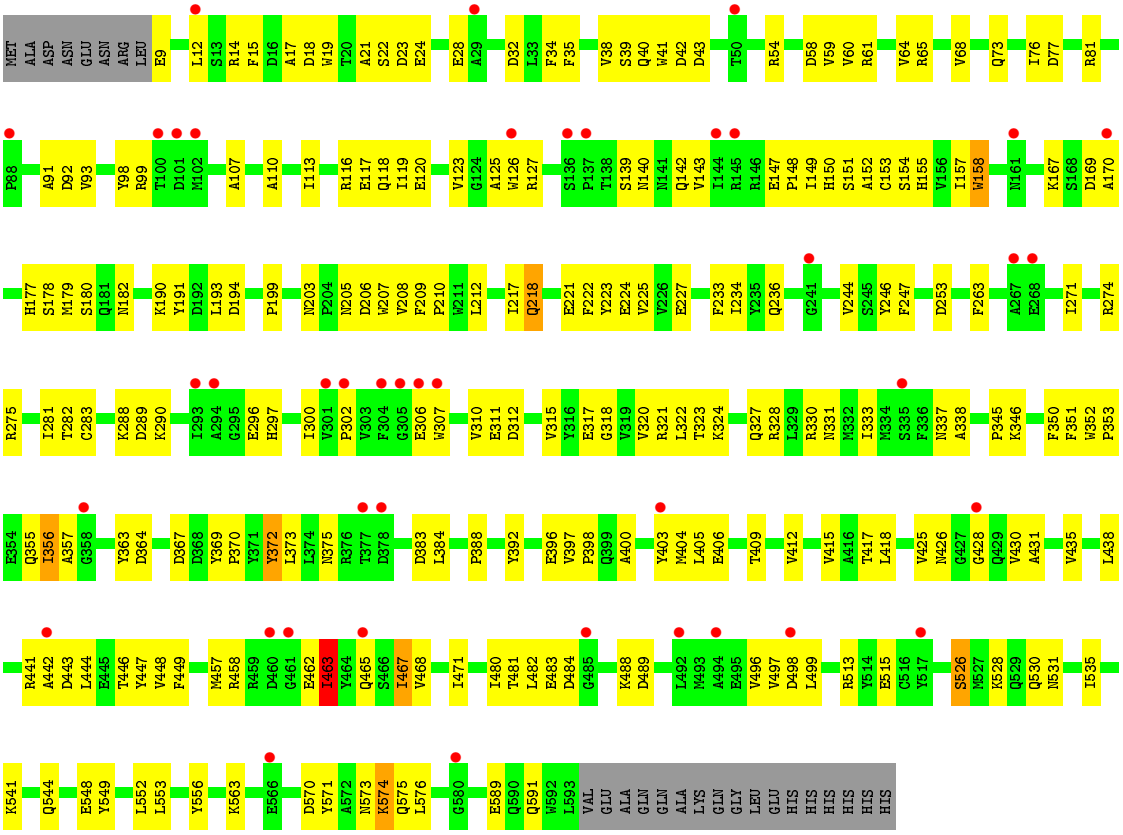
Chain E:





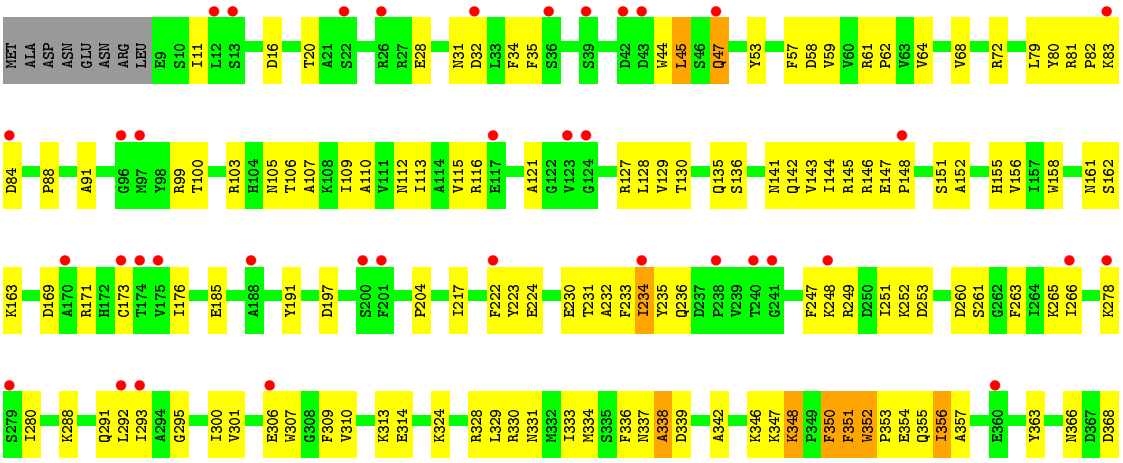
• Molecule 1: Portal protein

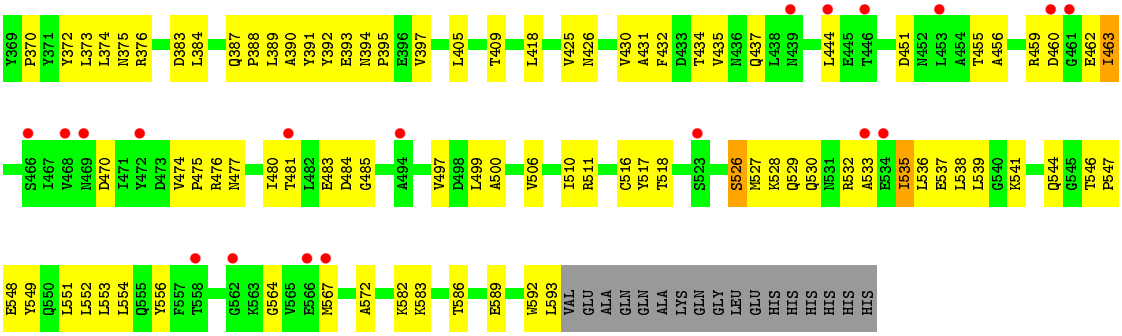
Chain F:



• Molecule 1: Portal protein

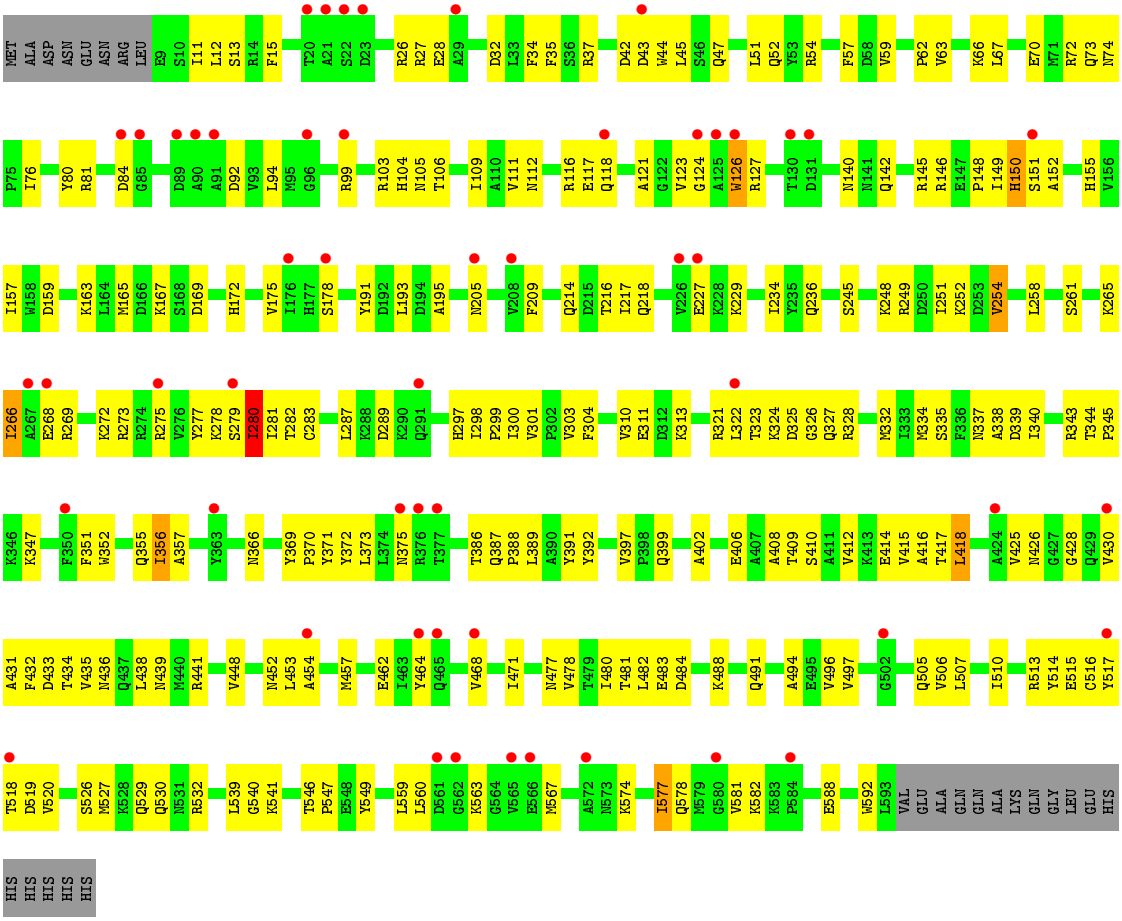
Chain G:





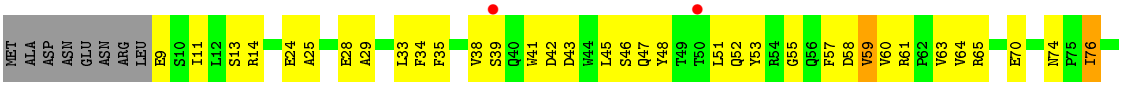
• Molecule 1: Portal protein

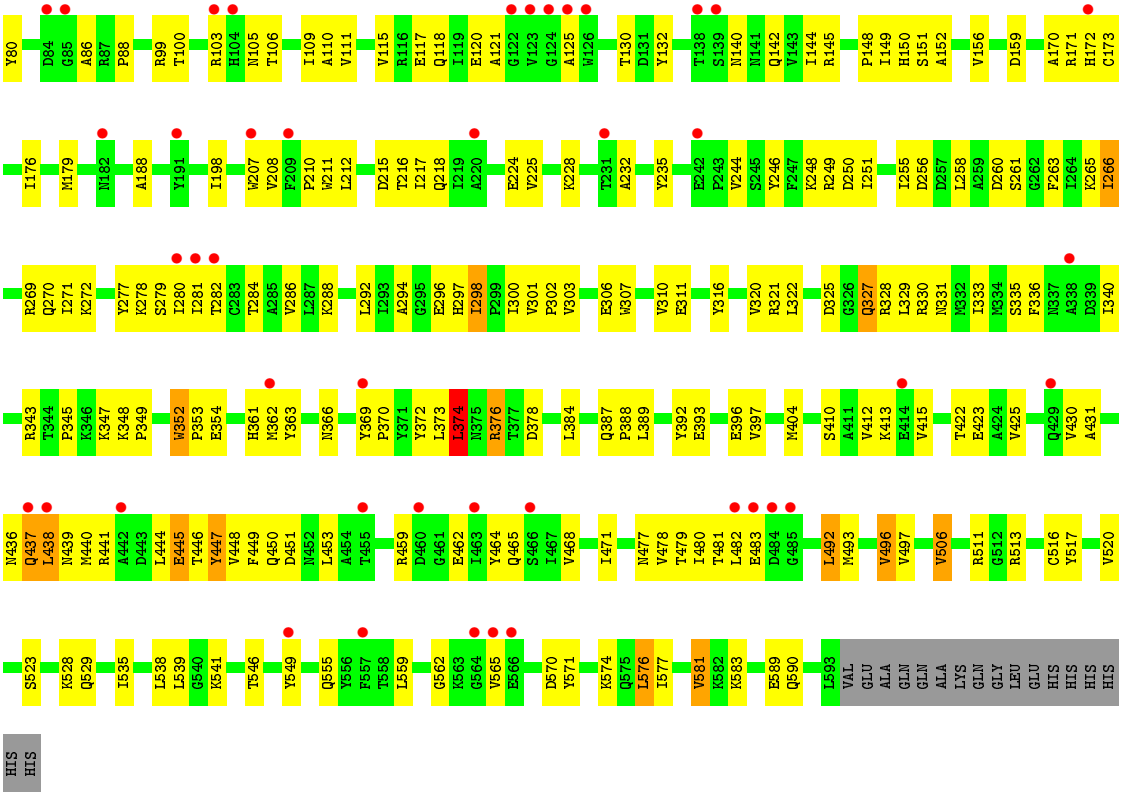
Chain H:



• Molecule 1: Portal protein

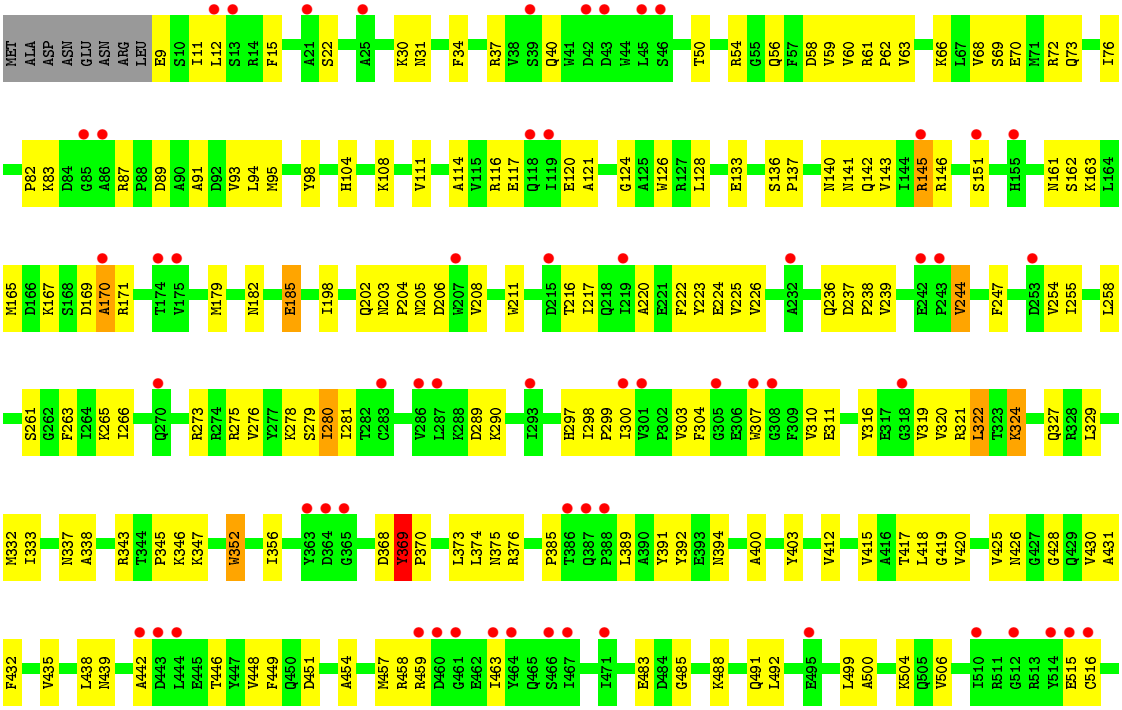
Chain I:

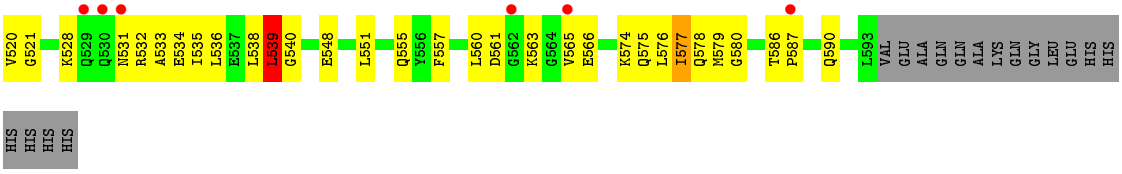




- Molecule 1: Portal protein

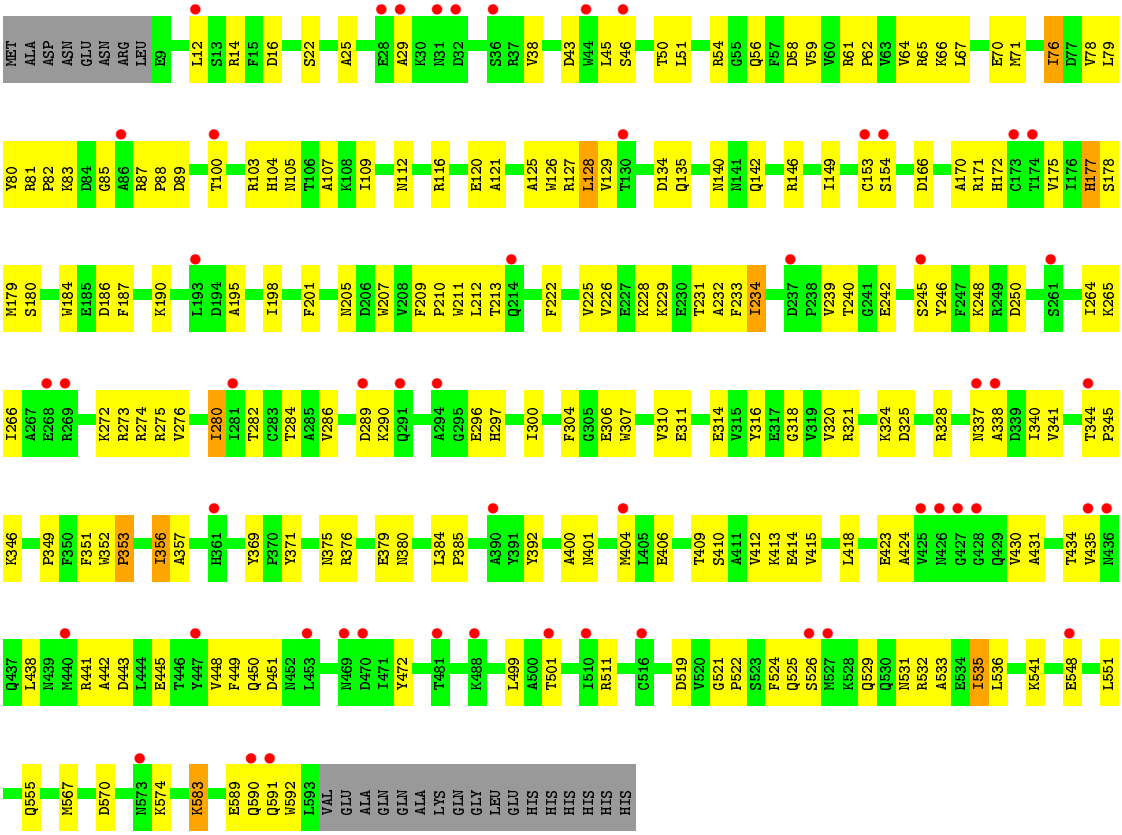
Chain J:





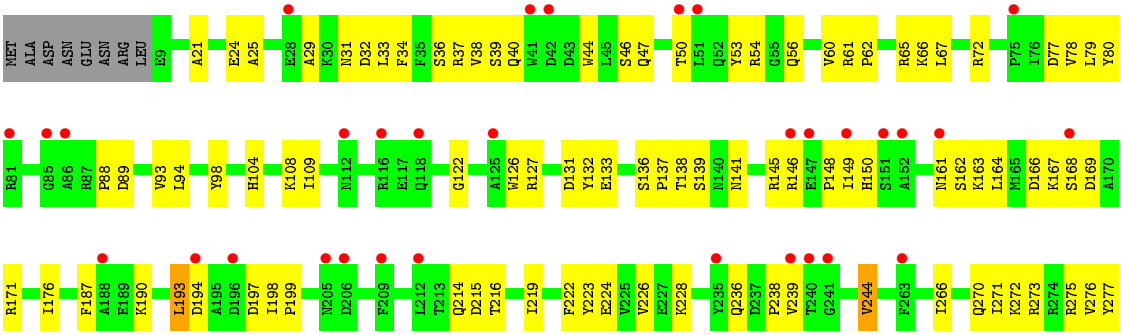
• Molecule 1: Portal protein

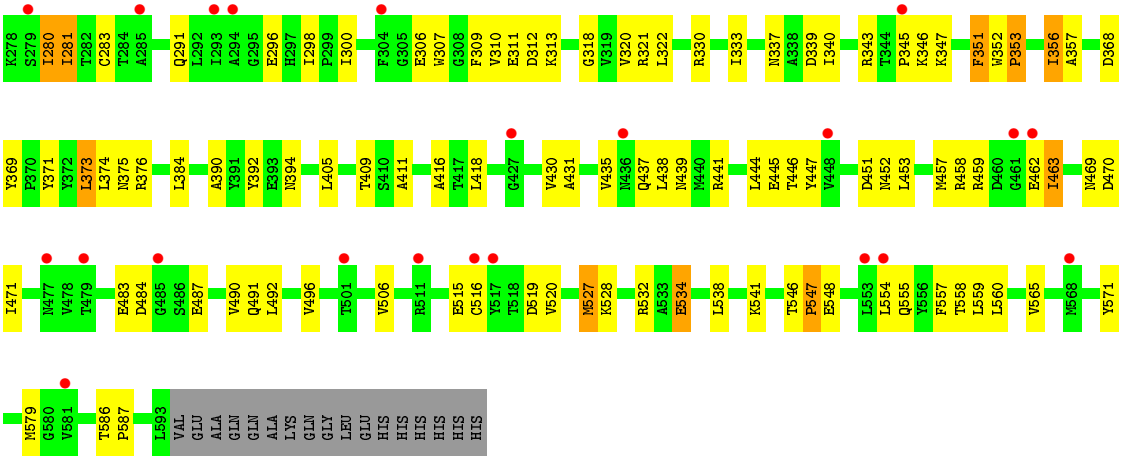
Chain K:



• Molecule 1: Portal protein

Chain L:




K278 S279 I280 I281 T282 C283 T284 A285
Q291 L292 I293 A294 G295 E296 H297 I298 P299 I300
F304 G305 E306 W307 G308 F309 V310 E311 D312 K313
G318 V319 V320 R321 L322
R330
I333
N337 A338 D339 I340
R343 T344 P345 K346 K347
F351 W352 P353
I356 A357
D368
Y369 P370 Y371 Y372 L373 L374 N375 R376
L384
A390 Y391 Y392 E393 N394
L405
T409 S410 A411
A416 T417 L418
G427
V430 A431
V435 N436 Q437 L438 N439 M440 R441
L444 E445 T446 Y447 V448
D451 N452 L453
M457 R458 R459
D460 G461 E462 I463
N469 D470
I471 N477 V478 T479
E483 D484 G485 S486 E487
V490 Q491 L492
V496
T501
V506
R511
E515 C516 Y517 T518 D519 V520
M527 K528
R532 A533 E534
L538
K541
T546 P547 E548
L553 L554 Q555 Y556 F557 T558 L559 L560
V565
M568
Y571
M579 G580 V581
T586 P587
L593 VAL GLU ALA GLN GLN ALA LYS GLN GLY LEU GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α, β, γ	316.81Å 316.81Å 138.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30 49.54 – 3.30	Depositor EDS
% Data completeness (in resolution range)	85.0 (15.00-3.30) 85.3 (49.54-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.295 , 0.315 0.309 , 0.322	Depositor DCC
R_{free} test set	1737 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	91.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 999.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-l	Xtriage
Reported twinning fraction	0.502 for H, K, L 0.498 for -H, K, -L	Depositor
Outliers	15 of 175831 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	56559	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/4826	0.58	0/6550
1	B	0.32	1/4812 (0.0%)	0.63	3/6533 (0.0%)
1	C	0.33	1/4812 (0.0%)	0.60	0/6533
1	D	0.30	0/4825	0.60	1/6550 (0.0%)
1	E	0.30	1/4822 (0.0%)	0.57	0/6546
1	F	0.28	0/4812	0.59	1/6533 (0.0%)
1	G	0.33	1/4808 (0.0%)	0.63	4/6528 (0.1%)
1	H	0.30	1/4812 (0.0%)	0.59	0/6533
1	I	0.30	1/4812 (0.0%)	0.61	3/6533 (0.0%)
1	J	0.30	1/4812 (0.0%)	0.59	1/6533 (0.0%)
1	K	0.28	0/4818	0.57	0/6541
1	L	0.28	0/4812	0.58	1/6533 (0.0%)
All	All	0.30	7/57783 (0.0%)	0.60	14/78446 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	6
1	C	0	8
1	D	0	11
1	E	0	9
1	F	0	10
1	G	0	7
1	H	0	8
1	I	0	8
1	J	0	10
1	K	0	7
1	L	0	7
All	All	0	96

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	348	LYS	C-N	9.99	1.53	1.34
1	E	203	ASN	C-N	8.28	1.50	1.34
1	H	352	TRP	C-N	8.19	1.49	1.34
1	J	203	ASN	C-N	7.31	1.48	1.34
1	I	298	ILE	C-N	5.64	1.45	1.34
1	B	80	TYR	C-N	5.05	1.45	1.34
1	G	353	PRO	N-CD	5.01	1.54	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	539	LEU	CA-CB-CG	7.27	132.03	115.30
1	D	192	ASP	N-CA-CB	-7.04	97.92	110.60
1	G	470	ASP	N-CA-C	6.31	128.03	111.00
1	I	492	LEU	CA-CB-CG	6.24	129.65	115.30
1	G	348	LYS	C-N-CD	6.21	141.43	128.40
1	G	470	ASP	CB-CA-C	-6.18	98.03	110.40
1	B	559	LEU	CA-CB-CG	6.01	129.12	115.30
1	G	352	TRP	C-N-CD	5.72	140.41	128.40
1	I	374	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	128	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	55	GLY	N-CA-C	5.42	126.65	113.10
1	L	193	LEU	CA-CB-CG	5.34	127.57	115.30
1	I	576	LEU	CA-CB-CG	5.24	127.36	115.30
1	F	463	ILE	CB-CA-C	-5.21	101.19	111.60

There are no chirality outliers.

All (96) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	SER	Peptide
1	A	177	HIS	Peptide
1	A	264	ILE	Peptide
1	A	352	TRP	Peptide
1	A	527	MET	Peptide
1	B	139	SER	Peptide
1	B	372	TYR	Peptide
1	B	41	TRP	Peptide
1	B	447	TYR	Peptide
1	B	54	ARG	Peptide
1	B	559	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	C	212	LEU	Peptide
1	C	226	VAL	Peptide
1	C	233	PHE	Peptide
1	C	369	TYR	Peptide
1	C	51	LEU	Peptide
1	C	587	PRO	Peptide
1	C	92	ASP	Peptide
1	C	93	VAL	Peptide
1	D	102	MET	Peptide
1	D	171	ARG	Peptide
1	D	191	TYR	Peptide
1	D	198	ILE	Peptide
1	D	206	ASP	Peptide
1	D	294	ALA	Peptide
1	D	511	ARG	Peptide
1	D	520	VAL	Peptide
1	D	527	MET	Peptide
1	D	558	THR	Peptide
1	D	582	LYS	Peptide
1	E	352	TRP	Peptide
1	E	370	PRO	Peptide
1	E	446	THR	Peptide
1	E	447	TYR	Peptide
1	E	452	ASN	Peptide
1	E	505	GLN	Peptide
1	E	53	TYR	Peptide
1	E	588	GLU	Peptide
1	E	79	LEU	Peptide
1	F	158	TRP	Peptide
1	F	167	LYS	Peptide
1	F	177	HIS	Peptide
1	F	218	GLN	Sidechain
1	F	315	VAL	Peptide
1	F	363	TYR	Peptide
1	F	364	ASP	Peptide
1	F	372	TYR	Peptide
1	F	526	SER	Peptide
1	F	574	LYS	Peptide
1	G	313	LYS	Peptide
1	G	363	TYR	Peptide
1	G	368	ASP	Peptide
1	G	45	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	G	47	GLN	Peptide
1	G	526	SER	Peptide
1	G	79	LEU	Peptide
1	H	126	TRP	Peptide
1	H	150	HIS	Peptide
1	H	159	ASP	Peptide
1	H	272	LYS	Peptide
1	H	280	ILE	Peptide
1	H	344	THR	Peptide
1	H	345	PRO	Peptide
1	H	530	GLN	Peptide
1	I	327	GLN	Sidechain
1	I	352	TRP	Peptide
1	I	376	ARG	Peptide
1	I	388	PRO	Peptide
1	I	41	TRP	Peptide
1	I	437	GLN	Sidechain
1	I	438	LEU	Peptide
1	I	445	GLU	Peptide
1	J	143	VAL	Peptide
1	J	145	ARG	Peptide
1	J	151	SER	Peptide
1	J	185	GLU	Peptide
1	J	322	LEU	Peptide
1	J	352	TRP	Peptide
1	J	368	ASP	Peptide
1	J	369	TYR	Peptide
1	J	454	ALA	Peptide
1	J	483	GLU	Peptide
1	K	128	LEU	Peptide
1	K	177	HIS	Peptide
1	K	201	PHE	Peptide
1	K	410	SER	Peptide
1	K	472	TYR	Peptide
1	K	526	SER	Peptide
1	K	583	LYS	Peptide
1	L	351	PHE	Peptide
1	L	368	ASP	Peptide
1	L	373	LEU	Peptide
1	L	527	MET	Peptide
1	L	534	GLU	Peptide
1	L	547	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	L	579	MET	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4724	0	4562	158	0
1	B	4710	0	4536	182	0
1	C	4710	0	4536	205	0
1	D	4723	0	4562	191	0
1	E	4720	0	4553	176	0
1	F	4710	0	4536	174	0
1	G	4706	0	4532	161	0
1	H	4710	0	4536	188	0
1	I	4710	0	4536	206	0
1	J	4710	0	4536	171	0
1	K	4716	0	4547	165	0
1	L	4710	0	4536	154	0
All	All	56559	0	54508	1959	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1959) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:297:HIS:HB3	1:I:450:GLN:OE1	1.30	1.26
1:I:447:TYR:OH	1:I:513:ARG:CD	1.88	1.21
1:I:447:TYR:OH	1:I:513:ARG:HD2	0.93	1.08
1:B:282:THR:OG1	1:B:285:ALA:O	1.85	0.95
1:I:297:HIS:CB	1:I:450:GLN:OE1	2.16	0.93
1:A:532:ARG:NH2	1:A:558:THR:OG1	2.02	0.93
1:D:290:LYS:HG3	1:D:290:LYS:O	1.69	0.91
1:I:446:THR:H	1:I:448:VAL:HG23	1.37	0.89
1:G:346:LYS:NZ	1:G:348:LYS:HG3	1.89	0.87
1:G:586:THR:OG1	1:G:589:GLU:OE2	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:MET:SD	1:A:505:GLN:NE2	2.47	0.86
1:G:235:TYR:O	1:G:236:GLN:HG2	1.76	0.84
1:L:44:TRP:O	1:L:47:GLN:NE2	2.09	0.84
1:H:337:ASN:OD1	1:H:338:ALA:N	2.11	0.84
1:H:178:SER:O	1:H:218:GLN:NE2	2.11	0.83
1:B:281:ILE:O	1:B:282:THR:OG1	1.96	0.83
1:C:42:ASP:OD2	1:C:44:TRP:NE1	2.12	0.83
1:I:297:HIS:ND1	1:I:450:GLN:HB2	1.94	0.83
1:L:131:ASP:OD2	1:L:291:GLN:NE2	2.11	0.83
1:B:532:ARG:NH2	1:B:558:THR:OG1	2.12	0.82
1:H:248:LYS:NZ	1:I:188:ALA:O	2.12	0.82
1:I:451:ASP:HB3	1:I:506:VAL:CA	2.10	0.81
1:I:447:TYR:CZ	1:I:513:ARG:HD2	2.12	0.81
1:E:237:ASP:OD2	1:E:240:THR:OG1	1.99	0.79
1:J:574:LYS:O	1:J:590:GLN:NE2	2.16	0.79
1:E:130:THR:OG1	1:E:189:GLU:OE2	2.01	0.78
1:K:414:GLU:OE2	1:L:330:ARG:NH2	2.17	0.78
1:I:327:GLN:HA	1:I:329:LEU:HG	1.65	0.78
1:B:463:ILE:HG22	1:B:463:ILE:O	1.83	0.78
1:J:343:ARG:NH1	1:L:369:TYR:OH	2.17	0.78
1:G:394:ASN:OD1	1:H:391:TYR:OH	2.01	0.77
1:L:104:HIS:O	1:L:145:ARG:NH1	2.17	0.77
1:J:208:VAL:O	1:J:211:TRP:NE1	2.17	0.77
1:C:325:ASP:HA	1:C:328:ARG:HG2	1.67	0.77
1:I:9:GLU:O	1:I:13:SER:OG	2.02	0.77
1:G:541:LYS:NZ	1:H:532:ARG:O	2.15	0.76
1:A:71:MET:SD	1:A:118:GLN:NE2	2.57	0.76
1:D:173:CYS:SG	1:D:174:THR:N	2.58	0.76
1:D:54:ARG:NE	1:D:334:MET:SD	2.60	0.75
1:I:321:ARG:O	1:J:56:GLN:NE2	2.18	0.75
1:G:141:ASN:ND2	1:G:451:ASP:OD1	2.18	0.75
1:F:81:ARG:NH1	1:F:515:GLU:O	2.20	0.74
1:F:463:ILE:O	1:F:463:ILE:HG22	1.87	0.74
1:C:545:GLY:O	1:C:549:TYR:N	2.20	0.74
1:G:549:TYR:O	1:G:553:LEU:N	2.20	0.74
1:A:478:VAL:O	1:A:479:THR:OG1	2.04	0.74
1:I:105:ASN:OD1	1:I:145:ARG:NH1	2.21	0.74
1:C:447:TYR:OH	1:C:516:CYS:O	2.05	0.73
1:D:476:ARG:HG2	1:D:477:ASN:H	1.53	0.73
1:E:54:ARG:NH2	1:E:335:SER:OG	2.20	0.73
1:E:161:ASN:OD1	1:E:163:LYS:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:GLU:O	1:F:321:ARG:NH1	2.22	0.73
1:F:77:ASP:OD1	1:F:98:TYR:OH	2.07	0.73
1:H:42:ASP:OD2	1:H:44:TRP:NE1	2.22	0.73
1:J:579:MET:SD	1:K:574:LYS:NZ	2.56	0.73
1:A:130:THR:HG21	1:A:186:ASP:HB2	1.71	0.72
1:B:451:ASP:OD1	1:B:506:VAL:N	2.23	0.72
1:D:149:ILE:HG22	1:D:150:HIS:H	1.54	0.72
1:A:392:TYR:HA	1:B:349:PRO:HG2	1.71	0.72
1:E:37:ARG:NH1	1:E:42:ASP:OD2	2.23	0.72
1:I:447:TYR:HH	1:I:513:ARG:HD2	1.49	0.72
1:I:159:ASP:OD1	1:J:182:ASN:ND2	2.22	0.71
1:J:15:PHE:HA	1:J:281:ILE:HD11	1.70	0.71
1:I:555:GLN:NE2	1:J:563:LYS:O	2.23	0.71
1:L:137:PRO:O	1:L:138:THR:OG1	2.06	0.71
1:D:198:ILE:HB	1:D:217:ILE:HD12	1.72	0.71
1:K:511:ARG:NH2	1:L:141:ASN:OD1	2.23	0.71
1:E:458:ARG:NH1	1:E:503:GLU:O	2.22	0.71
1:E:369:TYR:HB3	1:E:370:PRO:HD2	1.73	0.71
1:F:430:VAL:HG12	1:F:431:ALA:H	1.56	0.71
1:I:480:ILE:HG22	1:I:481:THR:H	1.54	0.71
1:E:488:LYS:NZ	1:E:495:GLU:OE2	2.17	0.71
1:B:569:ARG:O	1:B:574:LYS:NZ	2.24	0.71
1:F:352:TRP:NE1	1:F:375:ASN:O	2.24	0.71
1:D:319:VAL:O	1:E:61:ARG:NH1	2.24	0.70
1:C:149:ILE:HG22	1:C:150:HIS:H	1.57	0.70
1:D:345:PRO:O	1:D:348:LYS:NZ	2.25	0.70
1:I:451:ASP:HB3	1:I:506:VAL:N	2.07	0.70
1:K:179:MET:O	1:K:180:SER:OG	2.08	0.70
1:L:161:ASN:ND2	1:L:169:ASP:OD2	2.23	0.70
1:J:237:ASP:OD2	1:J:261:SER:OG	2.08	0.70
1:F:574:LYS:NZ	1:F:589:GLU:OE2	2.24	0.70
1:D:340:ILE:O	1:D:344:THR:OG1	2.10	0.70
1:B:451:ASP:OD2	1:B:513:ARG:NH1	2.25	0.69
1:F:337:ASN:OD1	1:F:338:ALA:N	2.24	0.69
1:I:316:TYR:O	1:J:40:GLN:NE2	2.21	0.69
1:G:510:ILE:HG22	1:G:511:ARG:H	1.58	0.69
1:G:88:PRO:HA	1:G:91:ALA:HB3	1.75	0.69
1:J:222:PHE:HB2	1:J:280:ILE:HG12	1.75	0.69
1:K:25:ALA:HA	1:K:29:ALA:HB3	1.75	0.69
1:J:133:GLU:OE2	1:J:140:ASN:ND2	2.25	0.69
1:L:280:ILE:O	1:L:281:ILE:HG22	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:GLY:O	1:E:462:GLU:HB2	1.92	0.69
1:E:526:SER:OG	1:F:563:LYS:NZ	2.26	0.68
1:I:297:HIS:HD1	1:I:450:GLN:HB2	1.56	0.68
1:G:530:GLN:HA	1:G:533:ALA:HB2	1.73	0.68
1:I:570:ASP:OD1	1:I:571:TYR:N	2.26	0.68
1:G:342:ALA:O	1:H:366:ASN:ND2	2.25	0.68
1:E:127:ARG:NH2	1:E:176:ILE:O	2.25	0.68
1:B:339:ASP:O	1:B:343:ARG:NH1	2.27	0.68
1:E:170:ALA:N	1:E:226:VAL:O	2.26	0.68
1:K:337:ASN:OD1	1:K:338:ALA:N	2.27	0.68
1:L:538:LEU:O	1:L:541:LYS:NZ	2.27	0.68
1:L:558:THR:O	1:L:560:LEU:N	2.27	0.67
1:B:443:ASP:OD2	1:B:446:THR:OG1	2.08	0.67
1:H:118:GLN:OE1	1:H:436:ASN:ND2	2.27	0.67
1:H:425:VAL:HG12	1:H:426:ASN:H	1.57	0.67
1:L:24:GLU:OE2	1:L:313:LYS:NZ	2.28	0.67
1:A:128:LEU:O	1:A:131:ASP:N	2.27	0.67
1:D:300:ILE:HG22	1:D:302:PRO:HD3	1.76	0.67
1:J:310:VAL:HG13	1:J:311:GLU:H	1.59	0.67
1:J:223:TYR:O	1:J:279:SER:OG	2.09	0.67
1:H:236:GLN:OE1	1:H:245:SER:OG	2.13	0.67
1:H:321:ARG:NH1	1:I:55:GLY:O	2.23	0.67
1:H:477:ASN:OD1	1:H:478:VAL:N	2.26	0.67
1:C:14:ARG:NH2	1:C:278:LYS:O	2.28	0.66
1:L:25:ALA:O	1:L:29:ALA:N	2.25	0.66
1:C:232:ALA:HB2	1:C:248:LYS:HA	1.77	0.66
1:G:337:ASN:OD1	1:G:338:ALA:N	2.28	0.66
1:J:179:MET:HE3	1:J:204:PRO:HD3	1.76	0.66
1:K:51:LEU:O	1:K:54:ARG:NH1	2.27	0.66
1:L:457:MET:HG3	1:L:458:ARG:H	1.61	0.66
1:F:570:ASP:OD1	1:F:571:TYR:N	2.29	0.66
1:I:171:ARG:HG2	1:I:224:GLU:HB3	1.76	0.66
1:K:50:THR:OG1	1:K:54:ARG:NH1	2.29	0.66
1:H:70:GLU:O	1:H:73:GLN:NE2	2.27	0.66
1:I:447:TYR:HE1	1:I:513:ARG:HG2	1.60	0.66
1:C:324:LYS:CD	1:D:57:PHE:HA	2.26	0.66
1:H:323:THR:OG1	1:H:414:GLU:OE1	2.14	0.66
1:L:32:ASP:OD1	1:L:122:GLY:N	2.29	0.65
1:B:280:ILE:HG13	1:B:281:ILE:H	1.61	0.65
1:B:57:PHE:HZ	1:B:327:GLN:HB3	1.61	0.65
1:E:427:GLY:N	1:E:429:GLN:OE1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:GLU:O	1:J:316:TYR:OH	2.13	0.65
1:E:414:GLU:O	1:E:417:THR:OG1	2.13	0.65
1:J:533:ALA:N	1:J:534:GLU:OE1	2.29	0.65
1:K:12:LEU:HB3	1:K:16:ASP:HB2	1.77	0.65
1:D:425:VAL:HG12	1:D:426:ASN:H	1.61	0.65
1:B:583:LYS:HD3	1:C:563:LYS:HB3	1.79	0.65
1:F:253:ASP:HB3	1:G:293:ILE:HD12	1.77	0.65
1:I:448:VAL:HG13	1:I:517:TYR:OH	1.96	0.65
1:K:103:ARG:HG2	1:K:104:HIS:H	1.60	0.65
1:G:375:ASN:OD1	1:G:376:ARG:N	2.30	0.65
1:H:559:LEU:HD12	1:H:560:LEU:N	2.12	0.65
1:J:117:GLU:HG3	1:J:121:ALA:HB3	1.78	0.65
1:J:216:THR:HG22	1:J:217:ILE:H	1.61	0.65
1:K:146:ARG:NH2	1:K:443:ASP:OD1	2.29	0.65
1:L:435:VAL:O	1:L:439:ASN:ND2	2.30	0.65
1:D:208:VAL:HG12	1:D:210:PRO:HD2	1.78	0.65
1:E:83:LYS:HG2	1:E:85:GLY:H	1.61	0.65
1:F:425:VAL:HG12	1:F:426:ASN:H	1.61	0.65
1:I:448:VAL:HG13	1:I:517:TYR:CZ	2.32	0.65
1:L:452:ASN:OD1	1:L:453:LEU:N	2.30	0.65
1:B:234:ILE:HG22	1:B:265:LYS:HE2	1.79	0.65
1:J:425:VAL:HG12	1:J:426:ASN:H	1.61	0.65
1:G:456:ALA:HB1	1:G:460:ASP:H	1.62	0.64
1:I:271:ILE:HG22	1:I:272:LYS:H	1.62	0.64
1:K:186:ASP:OD1	1:K:187:PHE:N	2.30	0.64
1:D:201:PHE:O	1:D:218:GLN:NE2	2.30	0.64
1:E:165:MET:HA	1:E:167:LYS:HD3	1.79	0.64
1:G:572:ALA:HB1	1:G:582:LYS:HD2	1.78	0.64
1:C:535:ILE:HG23	1:C:536:LEU:H	1.61	0.64
1:G:346:LYS:HZ2	1:G:348:LYS:HG3	1.62	0.64
1:K:310:VAL:HG12	1:K:311:GLU:HG2	1.79	0.64
1:C:369:TYR:HB3	1:C:371:TYR:HD2	1.63	0.64
1:L:21:ALA:O	1:L:313:LYS:NZ	2.30	0.64
1:A:443:ASP:OD1	1:A:444:LEU:N	2.31	0.64
1:K:126:TRP:HE1	1:K:146:ARG:HD3	1.63	0.64
1:J:352:TRP:HB3	1:J:374:LEU:HD22	1.80	0.64
1:C:171:ARG:NH2	1:C:296:GLU:OE1	2.31	0.64
1:A:203:ASN:OD1	1:A:204:PRO:HD2	1.98	0.63
1:B:36:SER:OG	1:B:120:GLU:O	2.15	0.63
1:C:65:ARG:NH1	1:C:69:SER:OG	2.31	0.63
1:G:346:LYS:HZ1	1:G:348:LYS:HG3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:VAL:HG23	1:J:280:ILE:HA	1.80	0.63
1:H:172:HIS:ND1	1:H:172:HIS:O	2.30	0.63
1:L:164:LEU:O	1:L:171:ARG:NH1	2.32	0.63
1:E:458:ARG:HH12	1:E:505:GLN:HG3	1.63	0.63
1:J:337:ASN:OD1	1:J:338:ALA:N	2.29	0.63
1:I:482:LEU:HG	1:I:483:GLU:H	1.64	0.63
1:J:457:MET:HG3	1:J:458:ARG:H	1.62	0.63
1:K:533:ALA:O	1:K:541:LYS:NZ	2.30	0.63
1:G:583:LYS:HB2	1:H:567:MET:HG2	1.81	0.63
1:F:467:ILE:HG22	1:F:468:VAL:HG23	1.81	0.63
1:B:216:THR:HG22	1:B:217:ILE:H	1.63	0.63
1:G:129:VAL:HG13	1:G:130:THR:HG23	1.81	0.63
1:I:297:HIS:HD1	1:I:450:GLN:CB	2.11	0.63
1:J:225:VAL:HG12	1:J:226:VAL:HG22	1.81	0.63
1:B:58:ASP:O	1:B:59:VAL:HG12	1.98	0.63
1:C:366:ASN:OD1	1:C:367:ASP:N	2.30	0.63
1:B:9:GLU:HG2	1:B:10:SER:H	1.64	0.62
1:C:248:LYS:O	1:C:249:ARG:HG2	1.99	0.62
1:G:547:PRO:HD2	1:H:549:TYR:HB2	1.80	0.62
1:H:441:ARG:NH2	1:H:517:TYR:O	2.31	0.62
1:J:11:ILE:O	1:J:278:LYS:NZ	2.31	0.62
1:I:451:ASP:HB3	1:I:506:VAL:CB	2.29	0.62
1:K:46:SER:OG	1:K:328:ARG:NH1	2.32	0.62
1:G:480:ILE:HG22	1:G:481:THR:H	1.63	0.62
1:J:289:ASP:OD1	1:J:290:LYS:N	2.32	0.62
1:L:375:ASN:OD1	1:L:376:ARG:N	2.31	0.62
1:A:167:LYS:HE2	1:A:169:ASP:HB2	1.80	0.62
1:E:138:THR:HG22	1:E:139:SER:H	1.64	0.62
1:F:118:GLN:HA	1:F:123:VAL:HG22	1.82	0.62
1:F:234:ILE:HD13	1:F:247:PHE:HB2	1.81	0.62
1:G:425:VAL:HG12	1:G:426:ASN:H	1.64	0.62
1:H:435:VAL:O	1:H:438:LEU:HB3	2.00	0.62
1:C:258:LEU:HD23	1:C:262:GLY:HA3	1.82	0.62
1:I:47:GLN:HG2	1:I:48:TYR:H	1.65	0.62
1:I:589:GLU:HG2	1:I:590:GLN:H	1.64	0.62
1:K:140:ASN:OD1	1:K:142:GLN:HB2	2.00	0.62
1:D:105:ASN:OD1	1:D:106:THR:N	2.33	0.62
1:F:355:GLN:HG2	1:F:373:LEU:HD11	1.82	0.62
1:L:62:PRO:O	1:L:66:LYS:NZ	2.33	0.62
1:K:226:VAL:O	1:K:226:VAL:HG12	1.99	0.62
1:F:179:MET:O	1:F:180:SER:OG	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:406:GLU:HA	1:H:409:THR:HG23	1.82	0.62
1:L:271:ILE:HG22	1:L:272:LYS:HG3	1.81	0.62
1:E:458:ARG:HG3	1:E:459:ARG:H	1.65	0.61
1:G:383:ASP:O	1:G:384:LEU:HD12	1.98	0.61
1:G:141:ASN:O	1:G:142:GLN:HG3	2.00	0.61
1:C:11:ILE:HG12	1:C:14:ARG:HE	1.65	0.61
1:C:543:PRO:HD3	1:D:532:ARG:HH22	1.64	0.61
1:D:290:LYS:CG	1:D:290:LYS:O	2.43	0.61
1:I:265:LYS:O	1:I:266:ILE:HG22	2.00	0.61
1:G:352:TRP:O	1:G:354:GLU:OE1	2.18	0.61
1:J:329:LEU:HA	1:J:332:MET:HB2	1.81	0.61
1:D:345:PRO:HB3	1:D:348:LYS:HE2	1.82	0.61
1:G:146:ARG:HG2	1:G:147:GLU:H	1.66	0.61
1:I:171:ARG:HD2	1:I:298:ILE:HD12	1.83	0.61
1:E:146:ARG:HH12	1:E:440:MET:HA	1.65	0.61
1:C:559:LEU:HD23	1:C:565:VAL:HG13	1.83	0.61
1:H:417:THR:OG1	1:I:65:ARG:NH1	2.34	0.61
1:J:258:LEU:HD22	1:J:263:PHE:HB3	1.82	0.61
1:A:322:LEU:HD11	1:A:411:ALA:HB1	1.81	0.61
1:A:43:ASP:OD1	1:A:43:ASP:N	2.34	0.61
1:E:312:ASP:OD1	1:E:313:LYS:N	2.34	0.61
1:F:544:GLN:OE1	1:G:544:GLN:NE2	2.34	0.61
1:B:312:ASP:OD2	1:C:211:TRP:NE1	2.19	0.60
1:B:215:ASP:OD1	1:B:216:THR:N	2.34	0.60
1:C:68:VAL:HA	1:C:71:MET:HB2	1.83	0.60
1:J:116:ARG:NH1	1:J:120:GLU:OE1	2.34	0.60
1:K:120:GLU:HG2	1:K:121:ALA:H	1.66	0.60
1:F:311:GLU:HG2	1:F:312:ASP:H	1.67	0.60
1:F:462:GLU:HG2	1:F:463:ILE:HG12	1.83	0.60
1:B:362:MET:HG2	1:B:366:ASN:HD21	1.67	0.60
1:E:231:THR:O	1:E:269:ARG:NH1	2.35	0.60
1:L:127:ARG:HB2	1:L:149:ILE:HA	1.83	0.60
1:H:149:ILE:HG13	1:H:150:HIS:H	1.66	0.60
1:H:34:PHE:HA	1:H:37:ARG:HG2	1.83	0.60
1:H:515:GLU:HG3	1:H:516:CYS:H	1.66	0.60
1:K:228:LYS:O	1:K:275:ARG:NH2	2.35	0.60
1:A:33:LEU:O	1:A:37:ARG:N	2.34	0.60
1:G:235:TYR:O	1:G:236:GLN:CG	2.50	0.60
1:B:573:ASN:OD1	1:B:574:LYS:NZ	2.34	0.60
1:I:336:PHE:HA	1:I:340:ILE:HG22	1.82	0.60
1:L:463:ILE:O	1:L:463:ILE:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLY:O	1:B:141:ASN:ND2	2.33	0.60
1:D:318:GLY:H	1:D:321:ARG:HH12	1.48	0.60
1:F:383:ASP:O	1:F:384:LEU:HD12	2.00	0.60
1:G:528:LYS:HE2	1:G:554:LEU:HD11	1.83	0.60
1:J:87:ARG:HG2	1:J:89:ASP:H	1.67	0.60
1:B:452:ASN:O	1:B:459:ARG:NH1	2.34	0.60
1:D:59:VAL:HG23	1:D:60:VAL:HG23	1.84	0.59
1:E:132:TYR:CE1	1:E:453:LEU:HD21	2.37	0.59
1:F:396:GLU:HG2	1:F:397:VAL:HG23	1.84	0.59
1:L:356:ILE:HG22	1:L:357:ALA:H	1.67	0.59
1:G:260:ASP:OD1	1:G:261:SER:N	2.35	0.59
1:I:42:ASP:OD1	1:I:43:ASP:N	2.33	0.59
1:K:175:VAL:HG23	1:K:177:HIS:CE1	2.37	0.59
1:D:376:ARG:NH1	1:D:377:THR:O	2.36	0.59
1:E:442:ALA:HA	1:E:445:GLU:HB2	1.84	0.59
1:C:321:ARG:O	1:D:56:GLN:NE2	2.35	0.59
1:G:280:ILE:HG12	1:G:288:LYS:HD3	1.83	0.59
1:H:248:LYS:O	1:H:249:ARG:HG2	2.02	0.59
1:H:287:LEU:HD23	1:H:289:ASP:H	1.67	0.59
1:L:36:SER:O	1:L:40:GLN:N	2.34	0.59
1:B:527:MET:HG3	1:B:528:LYS:H	1.67	0.59
1:B:541:LYS:HA	1:C:539:LEU:HD11	1.84	0.59
1:E:27:ARG:HG2	1:E:313:LYS:HD3	1.83	0.59
1:B:153:CYS:SG	1:B:154:SER:N	2.75	0.59
1:D:572:ALA:HA	1:D:575:GLN:HE22	1.67	0.59
1:E:478:VAL:HG12	1:E:479:THR:H	1.67	0.59
1:J:369:TYR:HB3	1:J:370:PRO:HD3	1.83	0.59
1:B:430:VAL:HG12	1:B:432:PHE:H	1.67	0.59
1:C:337:ASN:OD1	1:C:338:ALA:N	2.35	0.59
1:D:328:ARG:NE	1:E:53:TYR:OH	2.36	0.59
1:H:205:ASN:HB2	1:H:209:PHE:HA	1.84	0.59
1:A:231:THR:HG23	1:A:232:ALA:H	1.66	0.59
1:G:292:LEU:O	1:G:293:ILE:HD13	2.03	0.59
1:J:491:GLN:HG2	1:J:492:LEU:H	1.68	0.59
1:A:208:VAL:HG22	1:A:210:PRO:HD3	1.84	0.59
1:B:110:ALA:HB3	1:B:145:ARG:HH12	1.66	0.59
1:D:88:PRO:HG2	1:D:585:GLU:HB2	1.84	0.59
1:I:329:LEU:HD22	1:I:404:MET:HB3	1.84	0.59
1:I:437:GLN:NE2	1:I:520:VAL:HG13	2.18	0.59
1:J:223:TYR:C	1:J:280:ILE:HB	2.24	0.59
1:C:441:ARG:NH2	1:D:105:ASN:OD1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:448:VAL:HG13	1:I:517:TYR:CE1	2.38	0.58
1:B:81:ARG:HH12	1:B:518:THR:HA	1.69	0.58
1:B:535:ILE:HG22	1:B:539:LEU:HD13	1.84	0.58
1:J:319:VAL:HG23	1:J:320:VAL:H	1.67	0.58
1:J:528:LYS:HD3	1:J:531:ASN:HB3	1.85	0.58
1:F:199:PRO:HG2	1:F:218:GLN:HE21	1.68	0.58
1:H:165:MET:HG3	1:H:438:LEU:HD21	1.85	0.58
1:K:418:LEU:HA	1:L:66:LYS:HG2	1.84	0.58
1:E:340:ILE:O	1:E:344:THR:N	2.36	0.58
1:E:58:ASP:O	1:E:59:VAL:HG22	2.03	0.58
1:G:44:TRP:CD1	1:G:47:GLN:HG2	2.38	0.58
1:G:81:ARG:HH12	1:H:563:LYS:HB2	1.69	0.58
1:H:63:VAL:HG13	1:H:415:VAL:HG11	1.83	0.58
1:D:289:ASP:OD1	1:D:290:LYS:N	2.36	0.58
1:G:163:LYS:HG2	1:H:149:ILE:HG22	1.85	0.58
1:H:323:THR:HG23	1:H:412:VAL:HG13	1.84	0.58
1:H:480:ILE:HG13	1:H:481:THR:H	1.67	0.58
1:L:483:GLU:HG2	1:L:484:ASP:H	1.68	0.58
1:D:104:HIS:NE2	1:D:145:ARG:O	2.37	0.58
1:D:15:PHE:HZ	1:D:19:TRP:HE3	1.51	0.58
1:L:534:GLU:OE1	1:L:534:GLU:N	2.36	0.58
1:B:224:GLU:HB2	1:B:227:GLU:HG2	1.86	0.58
1:G:100:THR:OG1	1:G:103:ARG:NH2	2.36	0.58
1:I:130:THR:HG22	1:I:132:TYR:H	1.67	0.58
1:I:215:ASP:OD1	1:I:216:THR:N	2.36	0.58
1:J:141:ASN:OD1	1:J:141:ASN:O	2.21	0.58
1:I:111:VAL:HG22	1:I:439:ASN:HD21	1.69	0.58
1:J:265:LYS:O	1:J:266:ILE:HG22	2.04	0.58
1:A:353:PRO:HB3	1:A:356:ILE:HB	1.86	0.58
1:B:482:LEU:HG	1:B:483:GLU:H	1.67	0.58
1:E:378:ASP:OD1	1:E:379:GLU:N	2.37	0.58
1:K:525:GLN:N	1:K:529:GLN:OE1	2.32	0.58
1:G:231:THR:HG23	1:G:232:ALA:H	1.67	0.58
1:J:577:ILE:HG23	1:J:578:GLN:H	1.69	0.58
1:F:221:GLU:HB2	1:F:288:LYS:HE2	1.86	0.57
1:F:480:ILE:HG13	1:F:481:THR:H	1.69	0.57
1:H:356:ILE:HG12	1:H:357:ALA:H	1.69	0.57
1:K:58:ASP:OD2	1:K:61:ARG:NH1	2.37	0.57
1:D:558:THR:OG1	1:D:565:VAL:HG11	2.04	0.57
1:G:456:ALA:HB1	1:G:460:ASP:N	2.19	0.57
1:H:457:MET:HG2	1:H:505:GLN:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:379:GLU:HG3	1:K:380:ASN:H	1.69	0.57
1:D:401:ASN:HD22	1:D:405:LEU:HB2	1.68	0.57
1:E:425:VAL:HG13	1:E:536:LEU:HD21	1.86	0.57
1:G:328:ARG:HG2	1:G:329:LEU:H	1.69	0.57
1:I:269:ARG:HG2	1:I:270:GLN:H	1.68	0.57
1:K:356:ILE:HG13	1:K:357:ALA:N	2.20	0.57
1:F:125:ALA:HB3	1:F:149:ILE:HG13	1.85	0.57
1:H:51:LEU:HG	1:H:52:GLN:H	1.70	0.57
1:I:34:PHE:HB3	1:I:38:VAL:HG23	1.86	0.57
1:A:340:ILE:HD13	1:B:346:LYS:HD3	1.86	0.57
1:B:20:THR:O	1:B:24:GLU:N	2.33	0.57
1:B:383:ASP:O	1:B:384:LEU:HD12	2.04	0.57
1:K:67:LEU:HA	1:K:70:GLU:HB2	1.86	0.57
1:J:128:LEU:HD11	1:J:299:PRO:HB2	1.87	0.57
1:A:112:ASN:O	1:A:116:ARG:NH1	2.38	0.57
1:C:289:ASP:OD1	1:C:290:LYS:N	2.38	0.57
1:B:82:PRO:HB3	1:C:563:LYS:HG3	1.86	0.57
1:D:15:PHE:HA	1:D:18:ASP:HB2	1.87	0.57
1:G:11:ILE:HD12	1:G:278:LYS:HZ3	1.69	0.57
1:J:532:ARG:HH21	1:J:535:ILE:HG23	1.69	0.57
1:F:356:ILE:HG23	1:F:357:ALA:H	1.68	0.57
1:K:280:ILE:O	1:K:280:ILE:HG22	2.04	0.57
1:A:527:MET:HG3	1:A:559:LEU:HA	1.86	0.57
1:C:567:MET:HA	1:C:570:ASP:HB2	1.87	0.57
1:J:448:VAL:HG23	1:J:449:PHE:H	1.69	0.57
1:K:229:LYS:HD2	1:K:273:ARG:HH21	1.70	0.57
1:L:164:LEU:HD21	1:L:166:ASP:HB3	1.87	0.57
1:F:465:GLN:O	1:F:467:ILE:HG12	2.05	0.56
1:G:549:TYR:HA	1:G:552:LEU:HB2	1.87	0.56
1:K:340:ILE:O	1:K:344:THR:HG23	2.05	0.56
1:L:149:ILE:HG13	1:L:150:HIS:H	1.69	0.56
1:C:128:LEU:HD13	1:C:146:ARG:HE	1.69	0.56
1:C:167:LYS:HE2	1:C:445:GLU:HB3	1.86	0.56
1:H:167:LYS:HE3	1:H:169:ASP:HB2	1.85	0.56
1:B:546:THR:HB	1:B:547:PRO:HD3	1.85	0.56
1:I:140:ASN:OD1	1:I:142:GLN:NE2	2.38	0.56
1:J:346:LYS:HG3	1:K:369:TYR:HD2	1.71	0.56
1:F:369:TYR:HB2	1:F:370:PRO:HD3	1.86	0.56
1:F:351:PHE:HB2	1:F:388:PRO:HG2	1.88	0.56
1:J:142:GLN:OE1	1:J:142:GLN:N	2.39	0.56
1:C:323:THR:OG1	1:C:324:LYS:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:LYS:HD2	1:E:370:PRO:HB3	1.88	0.56
1:J:575:GLN:N	1:J:575:GLN:OE1	2.35	0.56
1:A:384:LEU:HD12	1:B:384:LEU:HG	1.86	0.56
1:I:523:SER:O	1:I:529:GLN:NE2	2.38	0.56
1:I:58:ASP:O	1:I:59:VAL:HG12	2.05	0.56
1:A:118:GLN:HG3	1:A:119:ILE:HD12	1.86	0.56
1:A:476:ARG:HG2	1:A:477:ASN:H	1.69	0.56
1:C:166:ASP:OD1	1:C:167:LYS:N	2.38	0.56
1:C:230:GLU:HG3	1:C:248:LYS:HD2	1.88	0.56
1:C:324:LYS:HD3	1:D:57:PHE:HA	1.87	0.56
1:E:127:ARG:HD2	1:E:149:ILE:HD12	1.88	0.56
1:I:156:VAL:HG22	1:I:176:ILE:HG23	1.87	0.56
1:J:280:ILE:HG13	1:J:281:ILE:N	2.20	0.56
1:L:280:ILE:HG12	1:L:281:ILE:H	1.71	0.56
1:D:534:GLU:O	1:D:537:GLU:N	2.35	0.56
1:L:351:PHE:HA	1:L:353:PRO:HD2	1.88	0.56
1:L:445:GLU:OE1	1:L:446:THR:HG23	2.06	0.56
1:C:356:ILE:HG12	1:C:357:ALA:H	1.71	0.56
1:F:157:ILE:HG22	1:F:158:TRP:H	1.70	0.56
1:F:320:VAL:O	1:F:324:LYS:NZ	2.29	0.56
1:H:34:PHE:HZ	1:H:45:LEU:HD21	1.70	0.56
1:J:297:HIS:NE2	1:J:451:ASP:O	2.38	0.56
1:K:125:ALA:H	1:K:149:ILE:HG12	1.70	0.56
1:L:215:ASP:O	1:L:216:THR:OG1	2.20	0.56
1:L:33:LEU:HD23	1:L:37:ARG:HH12	1.70	0.56
1:D:205:ASN:OD1	1:D:206:ASP:N	2.38	0.56
1:D:118:GLN:OE1	1:D:436:ASN:ND2	2.38	0.56
1:E:547:PRO:HG2	1:F:553:LEU:HD11	1.88	0.56
1:E:451:ASP:OD1	1:E:458:ARG:NH2	2.39	0.55
1:F:281:ILE:O	1:F:282:THR:OG1	2.24	0.55
1:G:389:LEU:HB2	1:H:389:LEU:HD21	1.88	0.55
1:I:441:ARG:HD3	1:I:444:LEU:HB3	1.88	0.55
1:K:375:ASN:OD1	1:K:376:ARG:N	2.39	0.55
1:C:120:GLU:N	1:C:120:GLU:OE1	2.40	0.55
1:D:171:ARG:NH1	1:D:173:CYS:H	2.04	0.55
1:A:68:VAL:HG11	1:L:431:ALA:HB2	1.88	0.55
1:L:469:ASN:OD1	1:L:470:ASP:N	2.40	0.55
1:A:452:ASN:ND2	1:A:506:VAL:O	2.40	0.55
1:E:322:LEU:HD22	1:F:59:VAL:HB	1.89	0.55
1:I:25:ALA:HA	1:I:28:GLU:HB2	1.89	0.55
1:C:117:GLU:N	1:C:117:GLU:OE1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:438:LEU:HD21	1:G:109:ILE:HG21	1.89	0.55
1:G:113:ILE:HD11	1:G:148:PRO:HB2	1.88	0.55
1:K:222:PHE:O	1:K:280:ILE:HG23	2.04	0.55
1:A:106:THR:HA	1:A:109:ILE:HG22	1.89	0.55
1:A:352:TRP:HE1	1:A:376:ARG:HH12	1.54	0.55
1:C:12:LEU:HD23	1:C:16:ASP:HB2	1.89	0.55
1:C:421:ASP:OD1	1:C:422:THR:N	2.37	0.55
1:I:477:ASN:OD1	1:I:478:VAL:N	2.39	0.55
1:A:81:ARG:HE	1:A:517:TYR:HB3	1.71	0.55
1:B:480:ILE:HG13	1:B:481:THR:H	1.69	0.55
1:B:82:PRO:O	1:B:83:LYS:HG3	2.06	0.55
1:B:526:SER:HB3	1:C:560:LEU:HD22	1.89	0.55
1:D:213:THR:O	1:D:214:GLN:HG2	2.07	0.55
1:D:77:ASP:OD1	1:D:78:VAL:N	2.40	0.55
1:F:142:GLN:O	1:F:143:VAL:HG13	2.06	0.55
1:E:415:VAL:HG11	1:F:59:VAL:HG23	1.89	0.55
1:H:369:TYR:HB2	1:H:370:PRO:HD3	1.88	0.55
1:J:347:LYS:HG2	1:J:391:TYR:CZ	2.42	0.55
1:I:541:LYS:HD3	1:J:532:ARG:NH2	2.21	0.55
1:I:431:ALA:HB2	1:J:72:ARG:HH22	1.71	0.55
1:D:306:GLU:OE2	1:D:315:VAL:N	2.39	0.55
1:D:485:GLY:O	1:D:488:LYS:NZ	2.31	0.55
1:H:15:PHE:HB3	1:H:281:ILE:HG21	1.88	0.55
1:H:298:ILE:HD12	1:H:298:ILE:O	2.07	0.55
1:C:199:PRO:HD2	1:C:219:ILE:HA	1.88	0.55
1:C:83:LYS:N	1:C:515:GLU:OE2	2.36	0.55
1:F:42:ASP:OD1	1:F:43:ASP:N	2.39	0.55
1:I:251:ILE:O	1:I:251:ILE:HG22	2.06	0.55
1:I:478:VAL:O	1:I:479:THR:HG23	2.07	0.55
1:L:228:LYS:O	1:L:273:ARG:NH2	2.28	0.55
1:L:39:SER:HB2	1:L:320:VAL:HG21	1.89	0.55
1:L:77:ASP:OD1	1:L:78:VAL:N	2.39	0.55
1:C:205:ASN:HD22	1:C:209:PHE:HB3	1.71	0.55
1:E:343:ARG:O	1:E:343:ARG:NH1	2.38	0.55
1:F:208:VAL:HG23	1:F:210:PRO:HD3	1.89	0.55
1:J:438:LEU:HD22	1:K:109:ILE:HG21	1.88	0.55
1:F:225:VAL:HG11	1:F:281:ILE:HD11	1.89	0.55
1:K:231:THR:HG23	1:K:232:ALA:H	1.69	0.55
1:A:25:ALA:HA	1:A:29:ALA:HB3	1.89	0.54
1:D:480:ILE:HG13	1:D:481:THR:H	1.73	0.54
1:E:301:VAL:N	1:E:302:PRO:HD3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:VAL:HG23	1:F:311:GLU:H	1.72	0.54
1:F:322:LEU:HD22	1:F:415:VAL:HB	1.89	0.54
1:G:80:TYR:HE1	1:G:444:LEU:HD21	1.71	0.54
1:H:546:THR:HB	1:H:547:PRO:HD3	1.89	0.54
1:B:15:PHE:O	1:B:19:TRP:N	2.38	0.54
1:B:25:ALA:HA	1:B:28:GLU:HG2	1.89	0.54
1:B:289:ASP:OD1	1:B:290:LYS:N	2.40	0.54
1:B:337:ASN:O	1:B:340:ILE:N	2.39	0.54
1:E:208:VAL:HG13	1:E:209:PHE:H	1.72	0.54
1:E:329:LEU:HD21	1:E:404:MET:HB2	1.89	0.54
1:E:546:THR:HB	1:E:547:PRO:HD3	1.90	0.54
1:K:296:GLU:HG3	1:K:297:HIS:ND1	2.22	0.54
1:L:390:ALA:O	1:L:394:ASN:ND2	2.40	0.54
1:A:297:HIS:HB2	1:A:446:THR:HB	1.89	0.54
1:E:141:ASN:OD1	1:E:455:THR:OG1	2.22	0.54
1:F:448:VAL:O	1:F:513:ARG:NH1	2.38	0.54
1:F:58:ASP:O	1:F:59:VAL:HG12	2.07	0.54
1:G:247:PHE:CE2	1:H:191:TYR:HA	2.43	0.54
1:G:309:PHE:HA	1:G:314:GLU:OE2	2.07	0.54
1:H:491:GLN:NE2	1:H:588:GLU:HA	2.22	0.54
1:H:577:ILE:HG23	1:H:578:GLN:H	1.72	0.54
1:I:151:SER:OG	1:I:152:ALA:N	2.40	0.54
1:I:581:VAL:HG23	1:I:583:LYS:H	1.72	0.54
1:J:321:ARG:H	1:K:61:ARG:HH22	1.54	0.54
1:A:190:LYS:HG3	1:A:191:TYR:H	1.73	0.54
1:F:126:TRP:HA	1:F:148:PRO:HA	1.90	0.54
1:K:38:VAL:HG21	1:K:321:ARG:HB2	1.89	0.54
1:A:249:ARG:HA	1:B:190:LYS:HE2	1.89	0.54
1:G:535:ILE:HG13	1:G:536:LEU:H	1.73	0.54
1:H:116:ARG:HG2	1:H:117:GLU:N	2.22	0.54
1:H:126:TRP:CZ2	1:H:152:ALA:HB3	2.43	0.54
1:H:322:LEU:HD22	1:H:414:GLU:HG3	1.88	0.54
1:I:430:VAL:HG22	1:I:431:ALA:H	1.73	0.54
1:L:127:ARG:HH11	1:L:150:HIS:HB2	1.72	0.54
1:B:463:ILE:CG2	1:B:463:ILE:O	2.55	0.54
1:C:324:LYS:HG2	1:D:56:GLN:HB3	1.89	0.54
1:C:82:PRO:HA	1:C:515:GLU:HG3	1.88	0.54
1:D:319:VAL:HG23	1:D:320:VAL:HG23	1.89	0.54
1:E:430:VAL:HG12	1:E:431:ALA:H	1.72	0.54
1:F:449:PHE:O	1:F:513:ARG:NH2	2.40	0.54
1:K:64:VAL:HG12	1:K:320:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:325:ASP:HA	1:L:56:GLN:HB3	1.90	0.54
1:K:79:LEU:HD13	1:K:525:GLN:HG3	1.90	0.54
1:E:14:ARG:NH1	1:E:225:VAL:HG22	2.22	0.54
1:I:447:TYR:HA	1:I:450:GLN:O	2.07	0.54
1:K:107:ALA:HB1	1:K:146:ARG:HG2	1.90	0.54
1:D:152:ALA:O	1:D:155:HIS:ND1	2.41	0.54
1:G:418:LEU:HD23	1:G:430:VAL:HG21	1.90	0.54
1:G:484:ASP:OD1	1:G:485:GLY:N	2.40	0.54
1:H:265:LYS:O	1:H:266:ILE:HG13	2.07	0.54
1:G:356:ILE:HG23	1:G:357:ALA:H	1.74	0.54
1:H:67:LEU:HD21	1:H:416:ALA:HA	1.89	0.54
1:J:91:ALA:HA	1:J:95:MET:HG3	1.90	0.54
1:A:353:PRO:HB3	1:A:356:ILE:HD13	1.90	0.53
1:A:405:LEU:O	1:A:409:THR:OG1	2.16	0.53
1:A:452:ASN:OD1	1:A:508:ASN:ND2	2.39	0.53
1:C:438:LEU:O	1:C:442:ALA:N	2.41	0.53
1:D:104:HIS:CE1	1:D:107:ALA:HB3	2.43	0.53
1:J:222:PHE:HD1	1:J:280:ILE:HG21	1.73	0.53
1:K:400:ALA:O	1:K:404:MET:N	2.29	0.53
1:D:447:TYR:OH	1:D:515:GLU:OE1	2.19	0.53
1:G:529:GLN:O	1:G:533:ALA:N	2.41	0.53
1:H:59:VAL:O	1:H:327:GLN:NE2	2.42	0.53
1:A:251:ILE:HD13	1:B:294:ALA:HA	1.89	0.53
1:A:548:GLU:O	1:A:552:LEU:HB2	2.09	0.53
1:B:114:ALA:HB1	1:B:124:GLY:HA2	1.89	0.53
1:G:191:TYR:OH	1:G:197:ASP:OD1	2.25	0.53
1:G:392:TYR:O	1:H:347:LYS:HG2	2.08	0.53
1:H:347:LYS:O	1:I:369:TYR:OH	2.27	0.53
1:I:431:ALA:HA	1:J:72:ARG:HH12	1.73	0.53
1:J:430:VAL:HG22	1:J:431:ALA:H	1.73	0.53
1:E:514:TYR:HE1	1:E:517:TYR:HB2	1.73	0.53
1:D:577:ILE:HD11	1:E:593:LEU:HD22	1.91	0.53
1:F:21:ALA:O	1:F:24:GLU:HG2	2.08	0.53
1:H:310:VAL:HG23	1:H:311:GLU:H	1.72	0.53
1:K:166:ASP:OD1	1:K:441:ARG:NH2	2.41	0.53
1:L:222:PHE:CG	1:L:281:ILE:HG21	2.43	0.53
1:L:527:MET:HE1	1:L:558:THR:O	2.08	0.53
1:F:498:ASP:OD1	1:F:499:LEU:N	2.42	0.53
1:F:528:LYS:HZ1	1:G:564:GLY:CA	2.20	0.53
1:J:528:LYS:NZ	1:J:557:PHE:O	2.36	0.53
1:K:14:ARG:HH11	1:K:226:VAL:HG21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLU:H	1:B:270:GLN:HE22	1.56	0.53
1:C:448:VAL:HG23	1:C:449:PHE:H	1.74	0.53
1:E:396:GLU:HG2	1:E:396:GLU:O	2.08	0.53
1:F:535:ILE:HD12	1:F:541:LYS:HB2	1.91	0.53
1:B:184:TRP:HB3	1:B:187:PHE:CE2	2.43	0.53
1:B:354:GLU:HB3	1:B:374:LEU:HA	1.90	0.53
1:D:187:PHE:O	1:D:190:LYS:N	2.41	0.53
1:D:394:ASN:HD22	1:E:389:LEU:HD11	1.74	0.53
1:F:288:LYS:HD2	1:F:288:LYS:H	1.72	0.53
1:H:510:ILE:HG22	1:H:510:ILE:O	2.09	0.53
1:J:22:SER:OG	1:J:202:GLN:OE1	2.17	0.53
1:J:327:GLN:OE1	1:J:327:GLN:N	2.41	0.53
1:C:400:ALA:HB2	1:D:398:PRO:HG2	1.91	0.53
1:C:477:ASN:OD1	1:C:478:VAL:N	2.42	0.53
1:D:137:PRO:O	1:D:138:THR:OG1	2.24	0.53
1:D:484:ASP:H	1:D:488:LYS:CE	2.22	0.53
1:I:100:THR:HA	1:I:103:ARG:HH21	1.74	0.53
1:K:384:LEU:HB3	1:K:385:PRO:HD2	1.91	0.53
1:L:223:TYR:CD2	1:L:224:GLU:HG2	2.44	0.53
1:B:558:THR:HG22	1:B:559:LEU:HD13	1.91	0.53
1:D:102:MET:O	1:D:103:ARG:NH1	2.37	0.53
1:D:130:THR:HG23	1:D:293:ILE:HG23	1.89	0.53
1:D:378:ASP:OD1	1:D:379:GLU:N	2.39	0.53
1:D:37:ARG:NH1	1:D:43:ASP:O	2.41	0.53
1:E:37:ARG:O	1:E:42:ASP:N	2.42	0.53
1:F:457:MET:HG3	1:F:458:ARG:H	1.73	0.53
1:G:437:GLN:NE2	1:G:518:THR:OG1	2.42	0.53
1:G:532:ARG:HH21	1:G:556:TYR:HA	1.73	0.53
1:I:451:ASP:HB3	1:I:506:VAL:HA	1.91	0.53
1:B:520:VAL:O	1:C:105:ASN:ND2	2.42	0.53
1:J:275:ARG:HG2	1:J:276:VAL:H	1.73	0.53
1:J:276:VAL:HG12	1:J:278:LYS:H	1.74	0.53
1:J:50:THR:OG1	1:J:54:ARG:NH1	2.42	0.53
1:L:236:GLN:HG3	1:L:238:PRO:HD3	1.91	0.53
1:A:462:GLU:C	1:A:463:ILE:HG13	2.30	0.52
1:I:172:HIS:NE2	1:I:300:ILE:O	2.31	0.52
1:K:61:ARG:HA	1:K:64:VAL:HG22	1.91	0.52
1:L:298:ILE:HD13	1:L:300:ILE:O	2.09	0.52
1:L:418:LEU:HD21	1:L:430:VAL:HG11	1.91	0.52
1:B:225:VAL:O	1:B:226:VAL:HG22	2.08	0.52
1:D:59:VAL:HB	1:D:324:LYS:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:PRO:CB	1:D:348:LYS:HE2	2.39	0.52
1:G:546:THR:HB	1:G:547:PRO:HD3	1.90	0.52
1:I:376:ARG:NH2	1:I:378:ASP:OD2	2.39	0.52
1:L:371:TYR:HE1	1:L:373:LEU:HD21	1.73	0.52
1:A:43:ASP:OD1	1:A:54:ARG:HD3	2.09	0.52
1:C:126:TRP:HA	1:C:149:ILE:HD12	1.89	0.52
1:I:373:LEU:HD23	1:I:373:LEU:O	2.09	0.52
1:I:80:TYR:HB2	1:I:516:CYS:HB3	1.91	0.52
1:K:280:ILE:CG2	1:K:280:ILE:O	2.57	0.52
1:K:296:GLU:HB2	1:K:451:ASP:OD1	2.09	0.52
1:D:187:PHE:CE1	1:D:190:LYS:HD3	2.43	0.52
1:D:222:PHE:CD2	1:D:280:ILE:HG12	2.45	0.52
1:F:571:TYR:HA	1:F:574:LYS:HE2	1.91	0.52
1:H:430:VAL:HG22	1:H:431:ALA:H	1.74	0.52
1:J:369:TYR:HB3	1:J:370:PRO:CD	2.39	0.52
1:K:352:TRP:N	1:K:353:PRO:HD3	2.24	0.52
1:L:353:PRO:HB3	1:L:373:LEU:HD22	1.90	0.52
1:L:532:ARG:NH2	1:L:555:GLN:OE1	2.41	0.52
1:H:74:ASN:ND2	1:H:433:ASP:OD1	2.41	0.52
1:K:442:ALA:HA	1:K:445:GLU:HG2	1.91	0.52
1:L:534:GLU:O	1:L:534:GLU:HG2	2.10	0.52
1:A:237:ASP:N	1:A:238:PRO:HD3	2.25	0.52
1:A:348:LYS:HB3	1:B:369:TYR:HB2	1.91	0.52
1:D:527:MET:HB3	1:D:559:LEU:HD13	1.92	0.52
1:K:170:ALA:HB2	1:K:297:HIS:HB3	1.90	0.52
1:B:107:ALA:HB1	1:B:145:ARG:HD3	1.92	0.52
1:D:239:VAL:HG13	1:D:240:THR:H	1.74	0.52
1:E:163:LYS:HE2	1:F:150:HIS:CE1	2.44	0.52
1:F:300:ILE:HG22	1:F:302:PRO:HD2	1.91	0.52
1:I:172:HIS:NE2	1:I:300:ILE:HG23	2.25	0.52
1:J:104:HIS:HB3	1:J:145:ARG:HD2	1.91	0.52
1:B:491:GLN:HG2	1:B:492:LEU:HD22	1.90	0.52
1:C:155:HIS:NE2	1:C:204:PRO:HD2	2.25	0.52
1:D:537:GLU:O	1:D:541:LYS:NZ	2.42	0.52
1:I:589:GLU:HG2	1:I:590:GLN:N	2.24	0.52
1:K:434:THR:OG1	1:L:72:ARG:NH2	2.43	0.52
1:L:281:ILE:O	1:L:281:ILE:HG23	2.10	0.52
1:C:111:VAL:O	1:C:115:VAL:HG23	2.10	0.52
1:C:309:PHE:HZ	1:C:315:VAL:O	1.92	0.52
1:D:506:VAL:HG12	1:D:507:LEU:N	2.25	0.52
1:H:34:PHE:CD1	1:H:37:ARG:HD3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:297:HIS:CE1	1:I:450:GLN:HB2	2.44	0.52
1:A:286:VAL:HG23	1:A:288:LYS:HG3	1.92	0.52
1:E:353:PRO:HB3	1:E:356:ILE:HD13	1.92	0.52
1:H:281:ILE:O	1:H:282:THR:OG1	2.26	0.52
1:J:31:ASN:HA	1:J:34:PHE:HB2	1.91	0.52
1:K:320:VAL:HG23	1:K:321:ARG:H	1.74	0.52
1:L:238:PRO:HG2	1:L:239:VAL:HG23	1.92	0.52
1:C:526:SER:OG	1:C:527:MET:N	2.43	0.51
1:D:209:PHE:CD1	1:D:210:PRO:HD3	2.45	0.51
1:E:208:VAL:HG22	1:E:210:PRO:HD3	1.92	0.51
1:F:127:ARG:N	1:F:147:GLU:O	2.43	0.51
1:F:443:ASP:O	1:F:446:THR:OG1	2.21	0.51
1:I:345:PRO:HB2	1:I:347:LYS:HG3	1.92	0.51
1:A:76:ILE:HG22	1:A:76:ILE:O	2.10	0.51
1:B:234:ILE:HG23	1:B:246:TYR:CD1	2.45	0.51
1:C:361:HIS:O	1:C:361:HIS:ND1	2.44	0.51
1:D:384:LEU:O	1:D:386:THR:N	2.42	0.51
1:E:522:PRO:HB2	1:E:524:PHE:CD2	2.45	0.51
1:F:190:LYS:HG2	1:F:191:TYR:H	1.75	0.51
1:K:76:ILE:HD12	1:K:521:GLY:O	2.09	0.51
1:L:40:GLN:HA	1:L:60:VAL:HG21	1.91	0.51
1:A:251:ILE:HG21	1:B:294:ALA:HB2	1.93	0.51
1:A:331:ASN:O	1:A:335:SER:N	2.39	0.51
1:D:45:LEU:N	1:D:47:GLN:OE1	2.43	0.51
1:E:379:GLU:HG2	1:E:380:ASN:H	1.75	0.51
1:F:571:TYR:O	1:F:574:LYS:HG2	2.10	0.51
1:G:28:GLU:O	1:G:32:ASP:N	2.42	0.51
1:H:268:GLU:HG2	1:H:269:ARG:HG2	1.93	0.51
1:K:43:ASP:O	1:K:45:LEU:HG	2.09	0.51
1:B:100:THR:HG22	1:B:141:ASN:HD21	1.75	0.51
1:B:70:GLU:O	1:B:73:GLN:NE2	2.42	0.51
1:F:306:GLU:O	1:F:307:TRP:HD1	1.93	0.51
1:H:163:LYS:HB3	1:H:167:LYS:HD2	1.92	0.51
1:I:39:SER:OG	1:I:120:GLU:OE2	2.28	0.51
1:I:492:LEU:HD13	1:I:493:MET:H	1.75	0.51
1:J:520:VAL:HG22	1:J:521:GLY:H	1.75	0.51
1:K:250:ASP:OD2	1:L:291:GLN:NE2	2.44	0.51
1:K:356:ILE:HG23	1:K:357:ALA:H	1.74	0.51
1:K:297:HIS:O	1:K:450:GLN:NE2	2.43	0.51
1:L:471:ILE:HG12	1:L:496:VAL:HG12	1.91	0.51
1:A:112:ASN:OD1	1:A:116:ARG:NH1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ARG:O	1:A:463:ILE:N	2.43	0.51
1:D:356:ILE:HG23	1:E:372:TYR:CE1	2.46	0.51
1:F:346:LYS:HB3	1:G:366:ASN:ND2	2.25	0.51
1:H:581:VAL:HG12	1:H:582:LYS:HD2	1.93	0.51
1:I:63:VAL:HG23	1:I:64:VAL:HG23	1.93	0.51
1:B:140:ASN:HA	1:B:454:ALA:HA	1.92	0.51
1:D:356:ILE:HG22	1:D:357:ALA:N	2.26	0.51
1:E:527:MET:HE3	1:E:560:LEU:HG	1.93	0.51
1:G:81:ARG:HD2	1:G:82:PRO:HD2	1.93	0.51
1:I:140:ASN:O	1:I:142:GLN:NE2	2.44	0.51
1:I:232:ALA:O	1:I:248:LYS:HE2	2.11	0.51
1:J:128:LEU:H	1:J:300:ILE:HG22	1.75	0.51
1:J:419:GLY:HA3	1:J:428:GLY:HA2	1.92	0.51
1:B:110:ALA:O	1:B:112:ASN:ND2	2.44	0.51
1:B:236:GLN:HB2	1:B:246:TYR:CE1	2.45	0.51
1:B:355:GLN:HB3	1:B:371:TYR:HE2	1.75	0.51
1:C:412:VAL:O	1:C:415:VAL:HG12	2.10	0.51
1:F:227:GLU:HA	1:F:275:ARG:HH22	1.76	0.51
1:G:80:TYR:CE1	1:G:444:LEU:HD21	2.46	0.51
1:I:447:TYR:CE1	1:I:513:ARG:HG2	2.44	0.51
1:I:528:LYS:HE2	1:J:563:LYS:HB3	1.93	0.51
1:J:531:ASN:ND2	1:J:555:GLN:HB3	2.26	0.51
1:C:281:ILE:HG22	1:C:281:ILE:O	2.10	0.51
1:D:127:ARG:HA	1:D:300:ILE:HG23	1.93	0.51
1:D:430:VAL:HG22	1:D:431:ALA:H	1.75	0.51
1:E:432:PHE:HA	1:E:435:VAL:HB	1.92	0.51
1:G:151:SER:OG	1:G:152:ALA:N	2.41	0.51
1:G:387:GLN:HG3	1:G:389:LEU:HD12	1.93	0.51
1:I:396:GLU:HG3	1:I:397:VAL:HG22	1.92	0.51
1:J:531:ASN:O	1:J:531:ASN:OD1	2.29	0.51
1:B:281:ILE:HG22	1:B:282:THR:HG23	1.93	0.51
1:H:26:ARG:HG2	1:H:27:ARG:H	1.75	0.51
1:J:304:PHE:O	1:J:439:ASN:ND2	2.33	0.51
1:K:430:VAL:HG12	1:K:431:ALA:H	1.75	0.51
1:B:129:VAL:HG13	1:B:143:VAL:HG13	1.93	0.51
1:E:315:VAL:HG12	1:E:316:TYR:CD2	2.46	0.51
1:H:94:LEU:HD13	1:H:94:LEU:O	2.10	0.51
1:I:374:LEU:HD13	1:I:374:LEU:H	1.76	0.51
1:H:322:LEU:HD23	1:I:59:VAL:HG23	1.93	0.51
1:J:225:VAL:HG23	1:J:280:ILE:CA	2.41	0.51
1:A:242:GLU:N	1:A:243:PRO:HD3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLN:HB2	1:B:246:TYR:CD1	2.46	0.50
1:B:461:GLY:O	1:B:462:GLU:HG2	2.10	0.50
1:C:165:MET:O	1:C:166:ASP:OD1	2.29	0.50
1:C:320:VAL:O	1:C:320:VAL:HG12	2.11	0.50
1:E:586:THR:HA	1:E:589:GLU:HB2	1.92	0.50
1:F:15:PHE:CE1	1:F:283:CYS:HB2	2.46	0.50
1:I:330:ARG:O	1:I:333:ILE:HG12	2.11	0.50
1:J:373:LEU:O	1:J:374:LEU:HD23	2.11	0.50
1:K:70:GLU:HG2	1:K:71:MET:HG3	1.93	0.50
1:A:388:PRO:HB3	1:B:352:TRP:CE3	2.46	0.50
1:B:170:ALA:HB2	1:B:227:GLU:HB2	1.94	0.50
1:C:15:PHE:HZ	1:C:225:VAL:HG11	1.75	0.50
1:D:161:ASN:OD1	1:D:163:LYS:NZ	2.21	0.50
1:D:324:LYS:HD2	1:D:327:GLN:HB2	1.92	0.50
1:G:173:CYS:HB2	1:G:301:VAL:HA	1.92	0.50
1:H:386:THR:HG22	1:H:388:PRO:HD3	1.92	0.50
1:I:448:VAL:CG1	1:I:517:TYR:CE1	2.95	0.50
1:L:244:VAL:O	1:L:244:VAL:HG12	2.11	0.50
1:L:199:PRO:HB3	1:L:283:CYS:HB3	1.93	0.50
1:A:126:TRP:CD1	1:A:300:ILE:HG23	2.46	0.50
1:B:21:ALA:HA	1:B:24:GLU:HG2	1.93	0.50
1:B:298:ILE:N	1:B:299:PRO:HD3	2.26	0.50
1:B:337:ASN:HA	1:B:340:ILE:HG22	1.92	0.50
1:F:296:GLU:HG3	1:F:297:HIS:N	2.26	0.50
1:G:143:VAL:O	1:G:144:ILE:HG23	2.11	0.50
1:A:59:VAL:HG22	1:L:322:LEU:HD22	1.92	0.50
1:E:529:GLN:O	1:E:533:ALA:N	2.44	0.50
1:H:408:ALA:HB1	1:H:412:VAL:HG23	1.94	0.50
1:I:260:ASP:OD1	1:I:261:SER:N	2.44	0.50
1:J:329:LEU:O	1:J:333:ILE:N	2.43	0.50
1:K:346:LYS:HG3	1:L:369:TYR:HB3	1.94	0.50
1:A:112:ASN:O	1:A:115:VAL:HG22	2.11	0.50
1:A:160:SER:OG	1:A:167:LYS:NZ	2.44	0.50
1:B:232:ALA:O	1:B:234:ILE:HG12	2.11	0.50
1:C:80:TYR:HB3	1:C:516:CYS:HB2	1.92	0.50
1:C:546:THR:CG2	1:C:547:PRO:HD3	2.41	0.50
1:F:496:VAL:HG23	1:F:497:VAL:H	1.76	0.50
1:G:222:PHE:O	1:G:280:ILE:HG22	2.12	0.50
1:H:418:LEU:HD21	1:H:428:GLY:O	2.11	0.50
1:I:255:ILE:HG22	1:I:256:ASP:N	2.26	0.50
1:J:205:ASN:O	1:J:206:ASP:OD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:529:GLN:O	1:K:532:ARG:O	2.29	0.50
1:L:554:LEU:HA	1:L:557:PHE:CE2	2.47	0.50
1:B:431:ALA:O	1:B:434:THR:HG22	2.11	0.50
1:C:58:ASP:O	1:C:59:VAL:HG12	2.12	0.50
1:I:412:VAL:O	1:I:415:VAL:HG12	2.12	0.50
1:L:164:LEU:HD22	1:L:168:SER:HB3	1.93	0.50
1:C:528:LYS:HB3	1:C:532:ARG:HH12	1.76	0.50
1:G:309:PHE:H	1:H:116:ARG:NH2	2.10	0.50
1:G:372:TYR:O	1:G:373:LEU:HB2	2.11	0.50
1:G:455:THR:HG23	1:G:456:ALA:H	1.75	0.50
1:H:397:VAL:O	1:H:399:GLN:N	2.45	0.50
1:A:126:TRP:HE1	1:A:128:LEU:HD11	1.77	0.50
1:D:340:ILE:HA	1:D:344:THR:HG23	1.94	0.50
1:D:570:ASP:OD1	1:D:573:ASN:ND2	2.29	0.50
1:E:306:GLU:OE1	1:E:306:GLU:N	2.45	0.50
1:G:110:ALA:HB1	1:G:148:PRO:HD3	1.93	0.50
1:H:165:MET:HE1	1:H:304:PHE:H	1.77	0.50
1:H:355:GLN:O	1:H:356:ILE:HG22	2.12	0.50
1:H:410:SER:O	1:H:414:GLU:N	2.42	0.50
1:H:62:PRO:O	1:H:66:LYS:NZ	2.38	0.50
1:K:531:ASN:OD1	1:K:532:ARG:N	2.42	0.50
1:C:173:CYS:HA	1:C:225:VAL:HG12	1.94	0.50
1:D:237:ASP:HB2	1:D:258:LEU:HD13	1.94	0.50
1:G:233:PHE:O	1:G:234:ILE:HB	2.12	0.50
1:G:405:LEU:O	1:G:409:THR:OG1	2.24	0.50
1:G:58:ASP:HB2	1:G:61:ARG:HH12	1.76	0.50
1:H:323:THR:O	1:H:327:GLN:N	2.42	0.50
1:I:438:LEU:HD22	1:I:440:MET:HB2	1.94	0.50
1:J:442:ALA:HA	1:K:104:HIS:CE1	2.47	0.50
1:A:28:GLU:HG3	1:A:313:LYS:HD2	1.94	0.49
1:J:223:TYR:CD2	1:J:224:GLU:HB3	2.47	0.49
1:L:167:LYS:NZ	1:L:296:GLU:O	2.35	0.49
1:B:348:LYS:HE3	1:B:350:PHE:HZ	1.77	0.49
1:C:132:TYR:HE1	1:C:455:THR:HG23	1.77	0.49
1:C:24:GLU:HA	1:C:28:GLU:HB3	1.93	0.49
1:C:485:GLY:O	1:C:488:LYS:NZ	2.38	0.49
1:C:589:GLU:OE1	1:C:589:GLU:N	2.45	0.49
1:D:123:VAL:HG11	1:D:155:HIS:CG	2.47	0.49
1:C:541:LYS:O	1:D:532:ARG:NH1	2.44	0.49
1:D:250:ASP:OD2	1:E:189:GLU:HG3	2.11	0.49
1:E:529:GLN:HB3	1:E:533:ALA:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:537:GLU:OE1	1:G:541:LYS:NZ	2.45	0.49
1:H:193:LEU:HD23	1:H:195:ALA:H	1.77	0.49
1:H:397:VAL:O	1:H:399:GLN:OE1	2.30	0.49
1:I:562:GLY:H	1:I:565:VAL:HB	1.77	0.49
1:I:76:ILE:HD13	1:I:437:GLN:HG3	1.93	0.49
1:L:21:ALA:HB1	1:L:313:LYS:HD3	1.93	0.49
1:A:80:TYR:HD1	1:A:516:CYS:HB3	1.76	0.49
1:D:15:PHE:HB2	1:D:281:ILE:HD12	1.93	0.49
1:G:291:GLN:O	1:G:292:LEU:HB2	2.13	0.49
1:F:323:THR:HG22	1:F:327:GLN:HG3	1.93	0.49
1:H:448:VAL:HG23	1:H:515:GLU:HB3	1.93	0.49
1:H:527:MET:O	1:H:529:GLN:N	2.46	0.49
1:H:514:TYR:CZ	1:I:103:ARG:HD2	2.48	0.49
1:I:11:ILE:HA	1:I:277:TYR:CE2	2.48	0.49
1:I:352:TRP:O	1:I:374:LEU:HB3	2.12	0.49
1:A:105:ASN:HB3	1:L:438:LEU:HD23	1.93	0.49
1:B:128:LEU:HD13	1:B:129:VAL:N	2.28	0.49
1:D:118:GLN:HG3	1:D:119:ILE:HD12	1.92	0.49
1:D:251:ILE:HG21	1:E:293:ILE:HG21	1.94	0.49
1:F:193:LEU:HD23	1:F:194:ASP:N	2.27	0.49
1:G:155:HIS:CD2	1:G:204:PRO:HD3	2.47	0.49
1:F:350:PHE:HE1	1:G:374:LEU:HB2	1.78	0.49
1:I:492:LEU:HD13	1:I:493:MET:N	2.27	0.49
1:J:300:ILE:O	1:J:300:ILE:HG13	2.13	0.49
1:B:441:ARG:NH1	1:B:518:THR:O	2.46	0.49
1:D:477:ASN:OD1	1:D:478:VAL:N	2.46	0.49
1:F:92:ASP:OD1	1:F:93:VAL:N	2.46	0.49
1:H:116:ARG:NH1	1:H:151:SER:HB2	2.28	0.49
1:H:99:ARG:NH1	1:H:103:ARG:HE	2.11	0.49
1:K:170:ALA:O	1:K:172:HIS:ND1	2.46	0.49
1:K:233:PHE:O	1:K:234:ILE:HG22	2.12	0.49
1:L:78:VAL:HB	1:L:519:ASP:HB3	1.94	0.49
1:A:222:PHE:CD2	1:A:279:SER:HB3	2.48	0.49
1:A:479:THR:HG22	1:A:480:ILE:N	2.28	0.49
1:B:270:GLN:O	1:B:271:ILE:HD13	2.13	0.49
1:B:271:ILE:HD12	1:B:275:ARG:NH2	2.28	0.49
1:D:527:MET:H	1:D:529:GLN:HG2	1.77	0.49
1:E:234:ILE:HG23	1:E:247:PHE:CE2	2.48	0.49
1:I:331:ASN:O	1:I:335:SER:N	2.45	0.49
1:J:70:GLU:OE2	1:J:428:GLY:HA3	2.13	0.49
1:A:552:LEU:HA	1:A:555:GLN:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ASP:CG	1:B:313:LYS:H	2.16	0.49
1:B:340:ILE:HG13	1:B:343:ARG:HB2	1.94	0.49
1:C:144:ILE:HG12	1:C:145:ARG:H	1.78	0.49
1:C:438:LEU:O	1:C:441:ARG:N	2.46	0.49
1:D:123:VAL:HG21	1:D:155:HIS:CE1	2.47	0.49
1:F:482:LEU:O	1:F:483:GLU:HG2	2.13	0.49
1:G:483:GLU:O	1:G:484:ASP:OD1	2.30	0.49
1:G:68:VAL:HG21	1:G:116:ARG:HH12	1.77	0.49
1:G:83:LYS:HG2	1:G:84:ASP:H	1.77	0.49
1:I:149:ILE:HG22	1:I:150:HIS:H	1.76	0.49
1:J:34:PHE:HA	1:J:37:ARG:HG2	1.95	0.49
1:D:123:VAL:HG13	1:D:303:VAL:HG22	1.95	0.49
1:E:216:THR:O	1:E:218:GLN:NE2	2.45	0.49
1:I:255:ILE:HD13	1:I:258:LEU:HD23	1.94	0.49
1:A:127:ARG:HH21	1:A:178:SER:H	1.60	0.49
1:C:400:ALA:O	1:C:403:TYR:N	2.44	0.49
1:E:369:TYR:HB3	1:E:370:PRO:CD	2.41	0.49
1:F:15:PHE:O	1:F:18:ASP:HB2	2.13	0.49
1:G:82:PRO:HB3	1:G:516:CYS:SG	2.53	0.49
1:I:441:ARG:O	1:I:444:LEU:HD23	2.13	0.49
1:K:65:ARG:HE	1:K:66:LYS:HE2	1.77	0.49
1:A:124:GLY:HA3	1:A:152:ALA:HB3	1.95	0.48
1:B:21:ALA:O	1:B:24:GLU:HG2	2.13	0.48
1:H:35:PHE:HD1	1:H:121:ALA:HA	1.78	0.48
1:I:250:ASP:OD1	1:I:250:ASP:N	2.46	0.48
1:J:68:VAL:HG13	1:J:69:SER:H	1.78	0.48
1:A:177:HIS:ND1	1:A:183:GLY:O	2.45	0.48
1:A:226:VAL:HG12	1:A:227:GLU:HG3	1.95	0.48
1:K:239:VAL:HG12	1:K:240:THR:N	2.28	0.48
1:K:239:VAL:HG12	1:K:240:THR:H	1.78	0.48
1:A:291:GLN:O	1:A:292:LEU:HB2	2.13	0.48
1:B:184:TRP:HB3	1:B:187:PHE:HE2	1.78	0.48
1:B:205:ASN:HD21	1:B:209:PHE:HA	1.77	0.48
1:B:279:SER:HB3	1:B:286:VAL:HG21	1.94	0.48
1:D:123:VAL:HG21	1:D:155:HIS:NE2	2.28	0.48
1:E:34:PHE:HB3	1:E:38:VAL:HG23	1.95	0.48
1:H:13:SER:OG	1:H:278:LYS:HG3	2.13	0.48
1:H:539:LEU:HD23	1:H:540:GLY:H	1.77	0.48
1:I:327:GLN:HA	1:I:329:LEU:CG	2.41	0.48
1:K:127:ARG:HD2	1:K:177:HIS:CG	2.48	0.48
1:L:340:ILE:HG22	1:L:343:ARG:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASN:OD1	1:A:376:ARG:N	2.46	0.48
1:A:503:GLU:OE1	1:A:503:GLU:N	2.45	0.48
1:C:265:LYS:O	1:C:266:ILE:HG22	2.14	0.48
1:C:557:PHE:HB2	1:C:568:MET:HG3	1.95	0.48
1:D:436:ASN:OD1	1:D:436:ASN:O	2.31	0.48
1:D:534:GLU:O	1:D:536:LEU:N	2.47	0.48
1:E:282:THR:HG22	1:E:283:CYS:N	2.28	0.48
1:E:430:VAL:HG12	1:E:431:ALA:N	2.29	0.48
1:E:450:GLN:N	1:E:450:GLN:OE1	2.45	0.48
1:E:57:PHE:O	1:E:59:VAL:HG13	2.13	0.48
1:F:118:GLN:HG3	1:F:119:ILE:HD12	1.95	0.48
1:F:153:CYS:SG	1:F:154:SER:N	2.86	0.48
1:F:43:ASP:HB2	1:F:328:ARG:NH2	2.29	0.48
1:G:161:ASN:OD1	1:G:162:SER:N	2.35	0.48
1:H:506:VAL:HA	1:H:513:ARG:HH21	1.79	0.48
1:K:225:VAL:HG22	1:K:226:VAL:HG23	1.96	0.48
1:K:413:LYS:HG3	1:K:414:GLU:HG3	1.96	0.48
1:K:59:VAL:O	1:K:59:VAL:HG12	2.13	0.48
1:A:225:VAL:HG22	1:A:226:VAL:HG23	1.95	0.48
1:B:584:PRO:HD3	1:C:567:MET:HE1	1.95	0.48
1:B:441:ARG:HG3	1:C:105:ASN:HB3	1.94	0.48
1:C:94:LEU:O	1:C:97:MET:N	2.43	0.48
1:D:471:ILE:HG23	1:D:472:TYR:H	1.79	0.48
1:G:499:LEU:HD13	1:G:500:ALA:N	2.29	0.48
1:I:340:ILE:O	1:I:343:ARG:HG2	2.14	0.48
1:L:266:ILE:O	1:L:266:ILE:HG12	2.13	0.48
1:C:249:ARG:NH2	1:C:251:ILE:HD11	2.29	0.48
1:D:329:LEU:HA	1:D:332:MET:HB2	1.95	0.48
1:D:360:GLU:HG2	1:D:361:HIS:ND1	2.28	0.48
1:E:333:ILE:HG22	1:E:333:ILE:O	2.13	0.48
1:F:212:LEU:HD12	1:F:212:LEU:O	2.13	0.48
1:H:527:MET:O	1:H:527:MET:HG3	2.13	0.48
1:I:328:ARG:HG2	1:I:328:ARG:O	2.14	0.48
1:H:321:ARG:NH2	1:I:58:ASP:OD2	2.47	0.48
1:K:109:ILE:HD12	1:K:112:ASN:HB2	1.95	0.48
1:K:116:ARG:NH1	1:K:120:GLU:HG3	2.28	0.48
1:L:462:GLU:O	1:L:463:ILE:HB	2.14	0.48
1:D:172:HIS:ND1	1:D:302:PRO:HG2	2.27	0.48
1:D:403:TYR:OH	1:E:398:PRO:HB2	2.13	0.48
1:F:99:ARG:HG2	1:F:99:ARG:O	2.13	0.48
1:G:263:PHE:HB3	1:G:265:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:310:VAL:HG13	1:I:311:GLU:H	1.78	0.48
1:I:322:LEU:HD12	1:J:61:ARG:HH11	1.79	0.48
1:I:438:LEU:HD11	1:I:520:VAL:HG21	1.96	0.48
1:K:187:PHE:O	1:K:190:LYS:N	2.33	0.48
1:B:319:VAL:HG23	1:B:320:VAL:HG13	1.96	0.48
1:C:533:ALA:O	1:C:535:ILE:HG22	2.13	0.48
1:F:428:GLY:O	1:F:430:VAL:HG23	2.13	0.48
1:I:277:TYR:CE2	1:I:279:SER:HB2	2.48	0.48
1:I:447:TYR:CE1	1:I:513:ARG:CG	2.97	0.48
1:A:479:THR:HG22	1:A:480:ILE:H	1.78	0.48
1:C:548:GLU:O	1:C:551:LEU:HB3	2.13	0.48
1:E:24:GLU:HB3	1:E:28:GLU:HB3	1.96	0.48
1:D:253:ASP:HB3	1:E:293:ILE:HG23	1.95	0.48
1:E:172:HIS:HB2	1:E:300:ILE:HG21	1.96	0.48
1:G:548:GLU:O	1:G:551:LEU:HB3	2.14	0.48
1:H:92:ASP:N	1:H:92:ASP:OD1	2.45	0.48
1:J:432:PHE:O	1:J:435:VAL:HG22	2.14	0.48
1:L:437:GLN:HG2	1:L:520:VAL:HG11	1.96	0.48
1:B:225:VAL:HG22	1:B:226:VAL:HG13	1.96	0.48
1:C:532:ARG:HE	1:C:558:THR:HG23	1.78	0.48
1:D:295:GLY:HA3	1:D:450:GLN:HG3	1.96	0.48
1:E:198:ILE:O	1:E:198:ILE:HG23	2.13	0.48
1:F:488:LYS:HG3	1:F:489:ASP:H	1.77	0.48
1:H:26:ARG:HH21	1:H:28:GLU:HB2	1.78	0.48
1:H:430:VAL:HG13	1:H:432:PHE:H	1.78	0.48
1:I:60:VAL:HG11	1:I:320:VAL:HG13	1.95	0.48
1:I:118:GLN:NE2	1:I:436:ASN:OD1	2.47	0.48
1:H:526:SER:HA	1:I:559:LEU:HD21	1.95	0.48
1:J:389:LEU:O	1:J:391:TYR:HD2	1.97	0.48
1:A:80:TYR:N	1:A:517:TYR:O	2.47	0.47
1:A:74:ASN:OD1	1:A:523:SER:OG	2.24	0.47
1:C:94:LEU:HD12	1:C:95:MET:N	2.29	0.47
1:D:31:ASN:OD1	1:D:32:ASP:N	2.47	0.47
1:E:282:THR:HG22	1:E:283:CYS:H	1.79	0.47
1:E:458:ARG:HD3	1:E:503:GLU:OE1	2.13	0.47
1:J:448:VAL:HG12	1:J:516:CYS:HB2	1.96	0.47
1:A:212:LEU:HD12	1:A:213:THR:N	2.28	0.47
1:B:509:ASP:HB3	1:C:137:PRO:O	2.15	0.47
1:D:114:ALA:HB2	1:D:148:PRO:HG3	1.95	0.47
1:D:527:MET:O	1:D:528:LYS:HB2	2.14	0.47
1:E:35:PHE:CG	1:E:36:SER:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:SER:HA	1:E:39:SER:HB3	1.96	0.47
1:G:324:LYS:HB2	1:H:54:ARG:NH1	2.29	0.47
1:K:448:VAL:HG23	1:K:449:PHE:H	1.78	0.47
1:B:123:VAL:HG12	1:B:124:GLY:H	1.77	0.47
1:C:128:LEU:HB2	1:C:146:ARG:HG2	1.96	0.47
1:C:478:VAL:C	1:C:479:THR:HG1	2.17	0.47
1:D:508:ASN:OD1	1:D:509:ASP:N	2.47	0.47
1:E:582:LYS:O	1:E:584:PRO:HD3	2.15	0.47
1:F:206:ASP:O	1:F:207:TRP:CD1	2.68	0.47
1:F:14:ARG:HB3	1:F:281:ILE:HD13	1.95	0.47
1:H:249:ARG:NH1	1:H:251:ILE:O	2.47	0.47
1:L:54:ARG:NH2	1:L:339:ASP:OD1	2.47	0.47
1:A:322:LEU:HB3	1:A:415:VAL:HG21	1.96	0.47
1:B:123:VAL:HG12	1:B:124:GLY:N	2.30	0.47
1:B:329:LEU:O	1:B:333:ILE:HG12	2.15	0.47
1:F:430:VAL:HG12	1:F:431:ALA:N	2.28	0.47
1:G:324:LYS:HB2	1:H:54:ARG:HH12	1.79	0.47
1:I:14:ARG:HB3	1:I:281:ILE:HG22	1.96	0.47
1:J:400:ALA:HA	1:J:403:TYR:CE2	2.49	0.47
1:J:58:ASP:OD2	1:J:61:ARG:NH1	2.32	0.47
1:L:318:GLY:O	1:L:321:ARG:NH1	2.48	0.47
1:A:327:GLN:N	1:A:327:GLN:OE1	2.48	0.47
1:B:587:PRO:O	1:B:588:GLU:HG3	2.14	0.47
1:B:68:VAL:HG21	1:B:116:ARG:HE	1.78	0.47
1:C:173:CYS:SG	1:C:174:THR:N	2.88	0.47
1:F:552:LEU:HD12	1:F:556:TYR:CE2	2.49	0.47
1:G:35:PHE:HB2	1:G:121:ALA:HA	1.96	0.47
1:G:480:ILE:HG22	1:G:481:THR:N	2.26	0.47
1:I:362:MET:HG3	1:I:363:TYR:CD2	2.49	0.47
1:I:372:TYR:CG	1:I:372:TYR:O	2.68	0.47
1:I:448:VAL:CG2	1:I:517:TYR:HE1	2.26	0.47
1:L:25:ALA:HB1	1:L:29:ALA:HB2	1.96	0.47
1:C:271:ILE:HD11	1:C:273:ARG:HH11	1.78	0.47
1:D:369:TYR:HB3	1:D:370:PRO:HD3	1.96	0.47
1:D:455:THR:OG1	1:D:456:ALA:N	2.45	0.47
1:E:351:PHE:HB2	1:E:388:PRO:HD3	1.96	0.47
1:E:37:ARG:HA	1:E:41:TRP:HB2	1.95	0.47
1:H:518:THR:HG22	1:H:519:ASP:H	1.80	0.47
1:I:325:ASP:H	1:J:56:GLN:HG2	1.80	0.47
1:B:434:THR:HA	1:B:437:GLN:OE1	2.15	0.47
1:C:109:ILE:HG13	1:C:110:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ASP:N	1:D:169:ASP:OD1	2.46	0.47
1:E:158:TRP:CZ2	1:E:174:THR:HG21	2.49	0.47
1:E:165:MET:HG3	1:E:304:PHE:HA	1.96	0.47
1:F:246:TYR:OH	1:F:274:ARG:NH2	2.48	0.47
1:F:397:VAL:N	1:F:398:PRO:HD3	2.30	0.47
1:G:395:PRO:HB2	1:G:397:VAL:HG23	1.96	0.47
1:K:242:GLU:HB3	1:K:245:SER:HA	1.97	0.47
1:L:44:TRP:CZ2	1:L:46:SER:HB2	2.50	0.47
1:F:61:ARG:HD2	1:F:65:ARG:HD2	1.96	0.47
1:H:117:GLU:HB3	1:H:121:ALA:HB3	1.95	0.47
1:H:328:ARG:O	1:H:332:MET:HG2	2.15	0.47
1:H:414:GLU:HG2	1:H:415:VAL:HG13	1.96	0.47
1:I:546:THR:O	1:I:549:TYR:HD2	1.98	0.47
1:J:273:ARG:HH11	1:J:275:ARG:HH22	1.62	0.47
1:B:558:THR:O	1:B:559:LEU:HD12	2.15	0.47
1:C:576:LEU:O	1:C:578:GLN:N	2.48	0.47
1:D:403:TYR:CZ	1:E:402:ALA:HB2	2.50	0.47
1:F:444:LEU:O	1:F:448:VAL:HG12	2.15	0.47
1:G:293:ILE:O	1:G:295:GLY:O	2.32	0.47
1:J:538:LEU:C	1:J:539:LEU:HD13	2.35	0.47
1:K:22:SER:HA	1:K:25:ALA:HB2	1.96	0.47
1:A:175:VAL:HG21	1:A:300:ILE:HD13	1.97	0.47
1:F:125:ALA:HB1	1:F:302:PRO:HB3	1.96	0.47
1:G:64:VAL:O	1:G:68:VAL:HG13	2.14	0.47
1:H:325:ASP:HB3	1:H:328:ARG:HE	1.80	0.47
1:J:63:VAL:HG11	1:J:321:ARG:HD3	1.97	0.47
1:J:412:VAL:HA	1:J:415:VAL:HG12	1.95	0.47
1:J:82:PRO:HB2	1:J:515:GLU:HG2	1.97	0.47
1:J:560:LEU:HG	1:J:561:ASP:H	1.79	0.47
1:K:499:LEU:HB3	1:K:501:THR:HG22	1.97	0.47
1:C:534:GLU:OE2	1:C:539:LEU:HG	2.16	0.47
1:D:462:GLU:OE1	1:D:464:TYR:HB2	2.15	0.47
1:F:330:ARG:O	1:F:333:ILE:HG12	2.15	0.47
1:E:348:LYS:HE3	1:F:370:PRO:O	2.15	0.47
1:F:9:GLU:OE1	1:F:9:GLU:N	2.47	0.47
1:H:42:ASP:OD1	1:H:43:ASP:N	2.40	0.47
1:J:30:LYS:HG2	1:J:34:PHE:CZ	2.50	0.47
1:I:322:LEU:HD12	1:J:61:ARG:HD2	1.96	0.47
1:J:63:VAL:HG21	1:J:321:ARG:NH2	2.30	0.47
1:K:280:ILE:HG21	1:K:286:VAL:HG11	1.96	0.47
1:K:567:MET:HA	1:K:570:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:SER:O	1:C:307:TRP:NE1	2.48	0.46
1:E:53:TYR:O	1:E:53:TYR:CD2	2.68	0.46
1:G:105:ASN:O	1:G:106:THR:HG22	2.14	0.46
1:G:328:ARG:HG2	1:G:329:LEU:N	2.29	0.46
1:G:53:TYR:HE2	1:G:339:ASP:HB2	1.80	0.46
1:J:565:VAL:HG12	1:J:565:VAL:O	2.15	0.46
1:L:271:ILE:HG22	1:L:272:LYS:N	2.30	0.46
1:L:418:LEU:HD21	1:L:430:VAL:HG21	1.97	0.46
1:A:574:LYS:H	1:A:577:ILE:HG23	1.80	0.46
1:C:206:ASP:OD1	1:C:210:PRO:HD3	2.15	0.46
1:E:432:PHE:HB3	1:E:436:ASN:HD22	1.81	0.46
1:F:12:LEU:HD12	1:F:12:LEU:O	2.15	0.46
1:G:72:ARG:HH21	1:G:116:ARG:HH21	1.64	0.46
1:I:249:ARG:HH21	1:I:251:ILE:HB	1.80	0.46
1:J:34:PHE:HD1	1:J:37:ARG:HD3	1.81	0.46
1:K:212:LEU:O	1:K:213:THR:HG22	2.15	0.46
1:B:296:GLU:OE1	1:B:296:GLU:N	2.47	0.46
1:D:356:ILE:HG22	1:D:357:ALA:H	1.81	0.46
1:E:306:GLU:HG2	1:E:306:GLU:O	2.16	0.46
1:F:14:ARG:HD2	1:F:17:ALA:HB3	1.97	0.46
1:F:236:GLN:HG2	1:F:263:PHE:CE1	2.51	0.46
1:G:432:PHE:O	1:G:435:VAL:HG12	2.16	0.46
1:H:124:GLY:HA2	1:H:303:VAL:H	1.80	0.46
1:H:84:ASP:HB2	1:I:99:ARG:HD2	1.97	0.46
1:K:318:GLY:O	1:L:61:ARG:NH1	2.48	0.46
1:K:583:LYS:NZ	1:L:565:VAL:HA	2.29	0.46
1:L:193:LEU:HD12	1:L:194:ASP:H	1.80	0.46
1:A:83:LYS:HG2	1:A:84:ASP:H	1.81	0.46
1:B:489:ASP:HB3	1:B:588:GLU:OE1	2.15	0.46
1:C:113:ILE:HB	1:C:116:ARG:HH12	1.81	0.46
1:E:362:MET:HE2	1:E:371:TYR:HB2	1.97	0.46
1:E:510:ILE:O	1:E:510:ILE:HG23	2.16	0.46
1:I:179:MET:SD	1:I:212:LEU:HB3	2.56	0.46
1:I:29:ALA:O	1:I:33:LEU:N	2.49	0.46
1:J:280:ILE:HG23	1:J:281:ILE:H	1.80	0.46
1:K:320:VAL:HG23	1:K:321:ARG:N	2.30	0.46
1:L:193:LEU:HD12	1:L:194:ASP:N	2.31	0.46
1:L:515:GLU:HG3	1:L:516:CYS:H	1.81	0.46
1:A:352:TRP:HE3	1:L:392:TYR:OH	1.99	0.46
1:A:61:ARG:NH1	1:L:321:ARG:HD2	2.31	0.46
1:B:531:ASN:ND2	1:B:555:GLN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:SER:HA	1:B:72:ARG:HH11	1.79	0.46
1:D:42:ASP:HB3	1:D:55:GLY:HA2	1.96	0.46
1:F:327:GLN:O	1:F:330:ARG:HG2	2.16	0.46
1:F:535:ILE:O	1:F:541:LYS:NZ	2.41	0.46
1:H:126:TRP:H	1:H:148:PRO:HB3	1.80	0.46
1:I:125:ALA:HB2	1:I:303:VAL:HG23	1.97	0.46
1:E:545:GLY:HA2	1:F:549:TYR:HD1	1.81	0.46
1:H:127:ARG:HH22	1:H:149:ILE:HD11	1.80	0.46
1:H:149:ILE:HG13	1:H:150:HIS:N	2.29	0.46
1:H:323:THR:HG22	1:H:327:GLN:HG2	1.97	0.46
1:H:577:ILE:HG23	1:H:578:GLN:N	2.30	0.46
1:I:142:GLN:HE21	1:I:453:LEU:HB3	1.81	0.46
1:J:111:VAL:HA	1:J:114:ALA:HB3	1.98	0.46
1:K:282:THR:HG22	1:K:284:THR:H	1.81	0.46
1:C:287:LEU:HD12	1:C:287:LEU:O	2.15	0.46
1:E:170:ALA:HA	1:E:227:GLU:HB3	1.97	0.46
1:E:362:MET:HG3	1:E:371:TYR:CG	2.50	0.46
1:F:223:TYR:CE1	1:F:224:GLU:HG2	2.51	0.46
1:F:548:GLU:O	1:F:552:LEU:HB2	2.15	0.46
1:F:169:ASP:OD2	1:G:185:GLU:HB3	2.16	0.46
1:I:310:VAL:HG13	1:I:311:GLU:N	2.31	0.46
1:J:346:LYS:HG3	1:K:369:TYR:CD2	2.50	0.46
1:K:522:PRO:HD2	1:K:524:PHE:HE2	1.80	0.46
1:A:513:ARG:O	1:A:514:TYR:HB2	2.16	0.46
1:B:216:THR:O	1:B:217:ILE:HG22	2.15	0.46
1:C:308:GLY:O	1:C:309:PHE:CG	2.69	0.46
1:E:215:ASP:OD1	1:E:216:THR:N	2.48	0.46
1:E:351:PHE:C	1:E:353:PRO:HD3	2.36	0.46
1:F:139:SER:OG	1:F:140:ASN:N	2.47	0.46
1:F:180:SER:HB3	1:F:182:ASN:H	1.81	0.46
1:F:323:THR:HA	1:F:412:VAL:HG12	1.97	0.46
1:H:249:ARG:HH12	1:H:254:VAL:HB	1.80	0.46
1:H:323:THR:O	1:H:326:GLY:N	2.48	0.46
1:J:321:ARG:HG3	1:J:322:LEU:H	1.81	0.46
1:K:345:PRO:O	1:K:392:TYR:OH	2.32	0.46
1:L:36:SER:HA	1:L:39:SER:HB3	1.98	0.46
1:B:179:MET:HB3	1:B:183:GLY:HA3	1.97	0.46
1:B:518:THR:HG23	1:B:520:VAL:H	1.81	0.46
1:C:15:PHE:CZ	1:C:225:VAL:HG11	2.51	0.46
1:D:128:LEU:HD23	1:D:129:VAL:O	2.16	0.46
1:E:300:ILE:HG22	1:E:300:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:PHE:HE1	1:F:151:SER:H	1.62	0.46
1:F:322:LEU:HD12	1:F:323:THR:OG1	2.16	0.46
1:H:574:LYS:O	1:H:592:TRP:NE1	2.49	0.46
1:I:110:ALA:HB1	1:I:148:PRO:HD2	1.98	0.46
1:I:496:VAL:HG13	1:I:497:VAL:N	2.31	0.46
1:K:423:GLU:CD	1:K:536:LEU:HD12	2.36	0.46
1:L:463:ILE:O	1:L:463:ILE:CG2	2.64	0.46
1:A:132:TYR:O	1:A:133:GLU:HG2	2.16	0.46
1:A:425:VAL:HG12	1:A:536:LEU:HD22	1.98	0.46
1:A:582:LYS:O	1:A:583:LYS:HD2	2.16	0.46
1:A:74:ASN:O	1:A:76:ILE:HG13	2.16	0.46
1:B:407:ALA:O	1:B:411:ALA:HB2	2.16	0.46
1:C:249:ARG:HD3	1:D:189:GLU:HG2	1.98	0.46
1:C:543:PRO:HG2	1:C:548:GLU:OE1	2.16	0.46
1:F:206:ASP:O	1:F:207:TRP:CG	2.69	0.46
1:F:327:GLN:O	1:F:331:ASN:ND2	2.48	0.46
1:F:438:LEU:O	1:F:441:ARG:HG2	2.16	0.46
1:G:128:LEU:H	1:G:300:ILE:CG2	2.29	0.46
1:G:110:ALA:CB	1:G:147:GLU:HA	2.44	0.46
1:G:330:ARG:O	1:G:333:ILE:HG12	2.16	0.46
1:G:99:ARG:O	1:G:103:ARG:HB2	2.15	0.46
1:H:172:HIS:CE1	1:H:175:VAL:HG22	2.51	0.46
1:I:45:LEU:HD12	1:I:46:SER:N	2.31	0.46
1:J:577:ILE:HG13	1:J:578:GLN:N	2.31	0.46
1:L:373:LEU:HD12	1:L:374:LEU:N	2.31	0.46
1:C:249:ARG:HH21	1:C:251:ILE:HD11	1.80	0.45
1:C:518:THR:HG23	1:C:520:VAL:HG23	1.98	0.45
1:D:163:LYS:HD2	1:E:149:ILE:HG12	1.98	0.45
1:F:40:GLN:HB3	1:F:41:TRP:HE3	1.81	0.45
1:H:57:PHE:O	1:H:59:VAL:HG13	2.15	0.45
1:J:60:VAL:HA	1:J:321:ARG:HH12	1.81	0.45
1:J:392:TYR:CG	1:J:392:TYR:O	2.70	0.45
1:A:337:ASN:HA	1:A:340:ILE:HG22	1.98	0.45
1:A:536:LEU:O	1:A:536:LEU:HD12	2.16	0.45
1:A:558:THR:HG22	1:A:559:LEU:HG	1.98	0.45
1:C:171:ARG:HG3	1:C:227:GLU:HA	1.99	0.45
1:C:280:ILE:HG23	1:C:281:ILE:H	1.81	0.45
1:C:535:ILE:HG23	1:C:536:LEU:N	2.31	0.45
1:E:312:ASP:CG	1:E:313:LYS:H	2.18	0.45
1:E:164:LEU:HD11	1:F:107:ALA:HB1	1.97	0.45
1:G:171:ARG:HG2	1:G:171:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:LYS:HE2	1:H:149:ILE:HB	1.98	0.45
1:H:559:LEU:HD13	1:H:560:LEU:O	2.16	0.45
1:I:117:GLU:O	1:I:121:ALA:N	2.36	0.45
1:H:356:ILE:HD11	1:I:372:TYR:CE2	2.52	0.45
1:K:134:ASP:OD1	1:K:135:GLN:N	2.48	0.45
1:L:47:GLN:HB3	1:L:50:THR:HG21	1.98	0.45
1:L:546:THR:OG1	1:L:547:PRO:HD3	2.16	0.45
1:A:187:PHE:O	1:A:190:LYS:NZ	2.40	0.45
1:B:112:ASN:OD1	1:B:113:ILE:N	2.50	0.45
1:B:437:GLN:HA	1:B:440:MET:HG2	1.98	0.45
1:D:98:TYR:HA	1:D:101:ASP:CG	2.37	0.45
1:D:401:ASN:ND2	1:D:405:LEU:HB2	2.30	0.45
1:F:438:LEU:HD11	1:G:109:ILE:HG22	1.99	0.45
1:G:169:ASP:O	1:G:171:ARG:N	2.49	0.45
1:I:198:ILE:HD12	1:I:217:ILE:HA	1.98	0.45
1:I:437:GLN:NE2	1:I:520:VAL:CG1	2.79	0.45
1:L:306:GLU:O	1:L:307:TRP:HD1	1.99	0.45
1:L:330:ARG:HA	1:L:333:ILE:HD12	1.98	0.45
1:A:337:ASN:OD1	1:A:338:ALA:N	2.49	0.45
1:C:525:GLN:HB2	1:C:529:GLN:OE1	2.17	0.45
1:D:329:LEU:O	1:D:332:MET:HB2	2.15	0.45
1:D:37:ARG:HH22	1:D:43:ASP:HA	1.82	0.45
1:D:451:ASP:HB3	1:D:506:VAL:H	1.82	0.45
1:E:161:ASN:OD1	1:E:162:SER:N	2.50	0.45
1:G:430:VAL:HG12	1:G:431:ALA:H	1.82	0.45
1:H:12:LEU:O	1:H:13:SER:OG	2.30	0.45
1:H:140:ASN:OD1	1:H:142:GLN:NE2	2.49	0.45
1:H:417:THR:O	1:H:418:LEU:HB2	2.16	0.45
1:I:144:ILE:HG22	1:I:145:ARG:N	2.31	0.45
1:K:280:ILE:HD12	1:K:286:VAL:HG21	1.97	0.45
1:A:21:ALA:HA	1:A:24:GLU:HG2	1.98	0.45
1:A:581:VAL:O	1:A:581:VAL:HG12	2.16	0.45
1:B:320:VAL:HG23	1:B:320:VAL:O	2.16	0.45
1:C:35:PHE:HZ	1:C:321:ARG:NH2	2.14	0.45
1:E:346:LYS:HD2	1:F:367:ASP:HB3	1.98	0.45
1:F:531:ASN:HB3	1:G:556:TYR:HE2	1.82	0.45
1:K:205:ASN:O	1:K:207:TRP:HE3	2.00	0.45
1:L:108:LYS:HG3	1:L:109:ILE:H	1.80	0.45
1:A:145:ARG:NH2	1:A:441:ARG:HE	2.15	0.45
1:A:232:ALA:O	1:A:234:ILE:HG12	2.16	0.45
1:C:387:GLN:OE1	1:D:385:PRO:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:N	1:C:62:PRO:HD3	2.32	0.45
1:D:350:PHE:HE1	1:D:363:TYR:HD2	1.63	0.45
1:D:164:LEU:HD12	1:E:147:GLU:OE1	2.17	0.45
1:E:311:GLU:O	1:E:312:ASP:OD1	2.34	0.45
1:F:322:LEU:HD12	1:F:323:THR:N	2.31	0.45
1:F:443:ASP:O	1:F:447:TYR:HD2	2.00	0.45
1:F:91:ALA:O	1:F:92:ASP:OD1	2.35	0.45
1:G:462:GLU:O	1:G:463:ILE:HG22	2.17	0.45
1:G:309:PHE:HB2	1:H:116:ARG:HH12	1.81	0.45
1:G:392:TYR:OH	1:H:351:PHE:HB3	2.17	0.45
1:J:280:ILE:HG13	1:J:281:ILE:H	1.81	0.45
1:L:270:GLN:O	1:L:271:ILE:HG13	2.17	0.45
1:L:88:PRO:O	1:L:89:ASP:OD1	2.34	0.45
1:A:458:ARG:O	1:A:459:ARG:HG3	2.16	0.45
1:A:538:LEU:HD13	1:A:541:LYS:HZ3	1.82	0.45
1:C:161:ASN:O	1:C:162:SER:OG	2.23	0.45
1:B:431:ALA:HB2	1:C:72:ARG:NH2	2.32	0.45
1:C:346:LYS:NZ	1:D:363:TYR:OH	2.50	0.45
1:E:145:ARG:NH2	1:E:147:GLU:OE2	2.49	0.45
1:F:169:ASP:OD1	1:F:170:ALA:N	2.41	0.45
1:F:34:PHE:O	1:F:38:VAL:HG22	2.17	0.45
1:F:400:ALA:O	1:F:404:MET:HG3	2.16	0.45
1:H:172:HIS:HB2	1:H:298:ILE:HD13	1.98	0.45
1:H:494:ALA:HB1	1:H:497:VAL:HG22	1.99	0.45
1:I:198:ILE:HG23	1:I:218:GLN:H	1.81	0.45
1:J:485:GLY:HA3	1:J:488:LYS:HE2	1.99	0.45
1:L:280:ILE:HG23	1:L:281:ILE:H	1.80	0.45
1:L:491:GLN:HG3	1:L:492:LEU:HD13	1.99	0.45
1:A:135:GLN:N	1:A:135:GLN:OE1	2.49	0.45
1:B:156:VAL:HG22	1:B:158:TRP:HE1	1.81	0.45
1:B:196:ASP:HB3	1:B:198:ILE:HG13	1.99	0.45
1:E:50:THR:O	1:E:51:LEU:HD12	2.17	0.45
1:F:468:VAL:O	1:F:468:VAL:HG12	2.17	0.45
1:I:263:PHE:HE2	1:I:265:LYS:HB2	1.82	0.45
1:I:14:ARG:O	1:I:281:ILE:HB	2.17	0.45
1:I:422:THR:O	1:I:423:GLU:HG2	2.16	0.45
1:J:198:ILE:HA	1:J:217:ILE:HG23	1.98	0.45
1:J:58:ASP:O	1:J:59:VAL:HG22	2.17	0.45
1:K:589:GLU:HG2	1:K:590:GLN:H	1.81	0.45
1:B:147:GLU:HG2	1:B:148:PRO:O	2.16	0.45
1:C:356:ILE:HG23	1:C:357:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:LEU:HD23	1:C:376:ARG:HH22	1.81	0.45
1:C:44:TRP:CD1	1:C:50:THR:HG21	2.51	0.45
1:C:579:MET:HE1	1:C:584:PRO:HD3	1.99	0.45
1:E:223:TYR:CD1	1:E:291:GLN:HB2	2.52	0.45
1:E:469:ASN:OD1	1:E:472:TYR:HB2	2.17	0.45
1:F:24:GLU:HB2	1:F:28:GLU:HB2	1.98	0.45
1:G:390:ALA:O	1:G:391:TYR:HB2	2.17	0.45
1:G:53:TYR:CE2	1:G:339:ASP:HB2	2.52	0.45
1:I:272:LYS:HG3	1:I:272:LYS:O	2.16	0.45
1:I:292:LEU:HD21	1:I:294:ALA:O	2.17	0.45
1:K:274:ARG:HH12	1:K:276:VAL:HG22	1.82	0.45
1:A:257:ASP:N	1:A:257:ASP:OD1	2.50	0.45
1:B:158:TRP:CD1	1:B:172:HIS:CE1	3.04	0.45
1:D:12:LEU:HD21	1:D:16:ASP:HB2	1.98	0.45
1:D:198:ILE:HG23	1:D:198:ILE:O	2.16	0.45
1:E:121:ALA:HB3	1:E:153:CYS:HB3	1.99	0.45
1:E:208:VAL:HG13	1:E:209:PHE:N	2.32	0.45
1:F:351:PHE:C	1:F:353:PRO:HD3	2.38	0.45
1:F:467:ILE:HG22	1:F:468:VAL:N	2.32	0.45
1:L:138:THR:HG22	1:L:139:SER:N	2.32	0.45
1:L:280:ILE:HG12	1:L:281:ILE:N	2.32	0.45
1:L:352:TRP:N	1:L:353:PRO:CD	2.80	0.45
1:B:236:GLN:HG3	1:B:237:ASP:OD1	2.17	0.44
1:D:451:ASP:OD2	1:D:459:ARG:NH2	2.42	0.44
1:E:106:THR:O	1:E:109:ILE:HG22	2.17	0.44
1:E:440:MET:HG3	1:E:440:MET:O	2.17	0.44
1:E:438:LEU:O	1:E:441:ARG:NH2	2.50	0.44
1:E:552:LEU:HA	1:E:556:TYR:CE2	2.52	0.44
1:F:589:GLU:HG3	1:F:591:GLN:HE22	1.82	0.44
1:G:355:GLN:O	1:G:356:ILE:HG22	2.17	0.44
1:H:273:ARG:HD3	1:H:275:ARG:HE	1.81	0.44
1:H:468:VAL:HG12	1:H:468:VAL:O	2.17	0.44
1:I:425:VAL:O	1:I:425:VAL:HG13	2.17	0.44
1:H:541:LYS:HE2	1:I:535:ILE:HG12	1.99	0.44
1:J:356:ILE:HD11	1:K:371:TYR:O	2.18	0.44
1:K:346:LYS:HB3	1:L:371:TYR:HE2	1.81	0.44
1:B:166:ASP:OD2	1:B:443:ASP:HA	2.18	0.44
1:B:441:ARG:NH2	1:B:518:THR:O	2.51	0.44
1:C:308:GLY:O	1:C:309:PHE:CD2	2.70	0.44
1:C:530:GLN:HA	1:C:533:ALA:HB2	1.99	0.44
1:F:110:ALA:O	1:F:113:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:TYR:CD2	1:G:224:GLU:HG3	2.52	0.44
1:I:352:TRP:NE1	1:I:376:ARG:HD2	2.33	0.44
1:I:459:ARG:HG3	1:I:462:GLU:HG2	1.98	0.44
1:I:70:GLU:OE1	1:I:70:GLU:N	2.48	0.44
1:K:184:TRP:HD1	1:K:187:PHE:CE2	2.35	0.44
1:B:170:ALA:O	1:B:171:ARG:HG2	2.17	0.44
1:B:581:VAL:HG12	1:B:582:LYS:N	2.32	0.44
1:C:163:LYS:NZ	1:C:314:GLU:OE2	2.38	0.44
1:C:350:PHE:CE1	1:C:353:PRO:HG3	2.53	0.44
1:C:407:ALA:HB1	1:D:330:ARG:HH12	1.82	0.44
1:C:479:THR:HG22	1:C:480:ILE:N	2.32	0.44
1:G:527:MET:HG3	1:G:527:MET:O	2.17	0.44
1:H:278:LYS:HD2	1:H:281:ILE:HD11	1.99	0.44
1:J:566:GLU:OE1	1:J:566:GLU:N	2.48	0.44
1:K:548:GLU:HA	1:K:551:LEU:HB3	1.98	0.44
1:L:136:SER:N	1:L:137:PRO:HD3	2.32	0.44
1:L:164:LEU:H	1:L:171:ARG:HH22	1.65	0.44
1:B:350:PHE:CZ	1:C:372:TYR:CE2	3.06	0.44
1:C:476:ARG:HG3	1:C:477:ASN:N	2.33	0.44
1:D:209:PHE:CG	1:D:210:PRO:HD3	2.52	0.44
1:E:196:ASP:O	1:E:198:ILE:HG22	2.17	0.44
1:E:83:LYS:HE3	1:E:85:GLY:HA3	2.00	0.44
1:F:415:VAL:HG12	1:F:415:VAL:O	2.17	0.44
1:G:251:ILE:HG13	1:G:253:ASP:H	1.82	0.44
1:H:453:LEU:HD23	1:H:454:ALA:H	1.82	0.44
1:J:254:VAL:HG23	1:J:255:ILE:N	2.33	0.44
1:L:36:SER:O	1:L:39:SER:N	2.50	0.44
1:L:487:GLU:O	1:L:490:VAL:HG12	2.17	0.44
1:A:557:PHE:HB3	1:A:568:MET:SD	2.57	0.44
1:B:252:LYS:NZ	1:B:256:ASP:OD1	2.45	0.44
1:B:447:TYR:HB2	1:B:449:PHE:H	1.82	0.44
1:B:544:GLN:NE2	1:B:552:LEU:HD12	2.33	0.44
1:C:206:ASP:N	1:C:206:ASP:OD1	2.51	0.44
1:C:280:ILE:HA	1:C:288:LYS:HE3	2.00	0.44
1:C:435:VAL:O	1:C:438:LEU:HD13	2.17	0.44
1:C:444:LEU:HD21	1:D:105:ASN:ND2	2.33	0.44
1:C:449:PHE:CD2	1:C:450:GLN:HG2	2.53	0.44
1:D:362:MET:HG3	1:D:373:LEU:HD21	1.99	0.44
1:D:440:MET:HG2	1:E:106:THR:HG22	1.98	0.44
1:E:402:ALA:HA	1:E:405:LEU:HG	1.99	0.44
1:E:447:TYR:HB3	1:E:450:GLN:OE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:ILE:HG22	1:I:150:HIS:N	2.31	0.44
1:K:209:PHE:N	1:K:210:PRO:HD3	2.33	0.44
1:A:436:ASN:HA	1:A:439:ASN:OD1	2.18	0.44
1:A:87:ARG:HG3	1:A:88:PRO:HD2	1.99	0.44
1:B:539:LEU:HG	1:B:540:GLY:H	1.81	0.44
1:C:341:VAL:HG23	1:C:342:ALA:N	2.33	0.44
1:C:560:LEU:O	1:C:565:VAL:HG11	2.17	0.44
1:C:61:ARG:HG3	1:C:320:VAL:HG11	1.98	0.44
1:C:63:VAL:HG22	1:C:67:LEU:HD13	1.99	0.44
1:D:276:VAL:HG11	1:D:278:LYS:HE3	2.00	0.44
1:D:419:GLY:HA3	1:D:428:GLY:HA2	1.98	0.44
1:H:299:PRO:O	1:H:301:VAL:HG23	2.18	0.44
1:H:356:ILE:HG23	1:H:357:ALA:N	2.33	0.44
1:H:462:GLU:O	1:H:464:TYR:HD2	2.01	0.44
1:I:28:GLU:HG3	1:I:29:ALA:H	1.83	0.44
1:I:384:LEU:HD11	1:J:385:PRO:HD3	1.99	0.44
1:I:496:VAL:HG22	1:I:497:VAL:H	1.82	0.44
1:I:496:VAL:HG13	1:I:497:VAL:H	1.82	0.44
1:K:211:TRP:CD1	1:K:212:LEU:HG	2.53	0.44
1:K:438:LEU:HD12	1:K:441:ARG:HH11	1.83	0.44
1:L:310:VAL:HG13	1:L:311:GLU:H	1.82	0.44
1:L:527:MET:HE3	1:L:528:LYS:H	1.82	0.44
1:A:75:PRO:HD2	1:A:523:SER:OG	2.18	0.44
1:C:17:ALA:HA	1:C:19:TRP:CE3	2.53	0.44
1:C:438:LEU:HD12	1:C:441:ARG:NH1	2.33	0.44
1:D:311:GLU:HG2	1:D:312:ASP:H	1.83	0.44
1:F:345:PRO:O	1:G:366:ASN:ND2	2.51	0.44
1:J:136:SER:N	1:J:137:PRO:HD3	2.32	0.44
1:J:179:MET:CE	1:J:204:PRO:HD3	2.46	0.44
1:J:375:ASN:OD1	1:J:376:ARG:N	2.48	0.44
1:K:128:LEU:HB3	1:K:300:ILE:HG22	1.99	0.44
1:L:280:ILE:HG23	1:L:281:ILE:N	2.33	0.44
1:A:161:ASN:HB2	1:A:167:LYS:HZ2	1.83	0.44
1:B:119:ILE:HG23	1:B:120:GLU:H	1.82	0.44
1:B:27:ARG:O	1:B:31:ASN:N	2.37	0.44
1:C:229:LYS:HD2	1:C:296:GLU:OE2	2.18	0.44
1:C:496:VAL:O	1:C:496:VAL:HG12	2.18	0.44
1:D:145:ARG:HG2	1:D:146:ARG:HG3	1.98	0.44
1:C:82:PRO:HD2	1:D:563:LYS:HE2	2.00	0.44
1:F:113:ILE:HD11	1:F:116:ARG:CZ	2.48	0.44
1:H:280:ILE:O	1:H:280:ILE:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:LEU:HD11	1:H:416:ALA:HA	2.00	0.44
1:J:70:GLU:OE1	1:J:73:GLN:NE2	2.50	0.44
1:K:423:GLU:CD	1:K:424:ALA:H	2.20	0.44
1:K:535:ILE:HG22	1:K:536:LEU:H	1.83	0.44
1:L:149:ILE:HG12	1:L:176:ILE:O	2.18	0.44
1:L:34:PHE:O	1:L:38:VAL:HG22	2.17	0.44
1:A:423:GLU:HG3	1:A:424:ALA:N	2.32	0.44
1:A:458:ARG:HG2	1:A:462:GLU:HG2	2.00	0.44
1:D:211:TRP:HE1	1:D:214:GLN:HG2	1.83	0.44
1:D:322:LEU:HD13	1:D:411:ALA:HB1	1.99	0.44
1:D:459:ARG:O	1:D:462:GLU:N	2.40	0.44
1:E:297:HIS:CE1	1:E:508:ASN:HB3	2.52	0.44
1:F:152:ALA:HA	1:F:155:HIS:CE1	2.52	0.44
1:F:244:VAL:HG13	1:F:244:VAL:O	2.18	0.44
1:F:23:ASP:OD1	1:F:24:GLU:N	2.51	0.44
1:F:54:ARG:NH1	1:F:331:ASN:O	2.51	0.44
1:F:417:THR:O	1:F:418:LEU:HD12	2.17	0.44
1:H:372:TYR:OH	1:H:375:ASN:OD1	2.18	0.44
1:H:436:ASN:ND2	1:H:439:ASN:OD1	2.35	0.44
1:I:144:ILE:CG2	1:I:145:ARG:N	2.81	0.44
1:K:171:ARG:HE	1:K:226:VAL:H	1.64	0.44
1:K:451:ASP:OD1	1:K:451:ASP:O	2.36	0.44
1:A:146:ARG:HH12	1:A:441:ARG:CZ	2.30	0.43
1:E:415:VAL:HG12	1:E:415:VAL:O	2.18	0.43
1:E:545:GLY:HA2	1:F:549:TYR:CD1	2.53	0.43
1:G:112:ASN:O	1:G:115:VAL:HG22	2.17	0.43
1:G:431:ALA:O	1:G:434:THR:OG1	2.26	0.43
1:H:126:TRP:CE2	1:H:152:ALA:HB3	2.53	0.43
1:K:198:ILE:O	1:K:198:ILE:HG23	2.18	0.43
1:K:351:PHE:O	1:K:352:TRP:HD1	2.01	0.43
1:L:275:ARG:HG2	1:L:276:VAL:N	2.32	0.43
1:B:439:ASN:HA	1:B:442:ALA:HB2	2.00	0.43
1:E:197:ASP:OD2	1:E:288:LYS:NZ	2.34	0.43
1:E:438:LEU:O	1:E:441:ARG:NE	2.50	0.43
1:F:14:ARG:O	1:F:17:ALA:HB3	2.18	0.43
1:F:373:LEU:O	1:F:373:LEU:HD12	2.18	0.43
1:F:65:ARG:HA	1:F:68:VAL:HG22	2.00	0.43
1:F:350:PHE:HZ	1:G:374:LEU:HD13	1.83	0.43
1:G:459:ARG:HG3	1:G:459:ARG:O	2.19	0.43
1:G:526:SER:HA	1:G:529:GLN:HB3	1.99	0.43
1:G:538:LEU:HB3	1:G:539:LEU:H	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:ASP:O	1:H:35:PHE:HD2	2.01	0.43
1:H:402:ALA:O	1:H:406:GLU:HG2	2.17	0.43
1:J:322:LEU:O	1:J:324:LYS:N	2.51	0.43
1:J:548:GLU:O	1:J:551:LEU:N	2.51	0.43
1:J:576:LEU:HB3	1:J:580:GLY:H	1.83	0.43
1:K:273:ARG:HD3	1:K:273:ARG:HA	1.81	0.43
1:K:555:GLN:OE1	1:K:555:GLN:N	2.50	0.43
1:A:208:VAL:HG13	1:A:209:PHE:N	2.33	0.43
1:A:437:GLN:HB2	1:B:109:ILE:HD11	2.00	0.43
1:B:234:ILE:HG23	1:B:246:TYR:CE1	2.53	0.43
1:B:354:GLU:HB2	1:B:375:ASN:H	1.83	0.43
1:B:87:ARG:O	1:B:87:ARG:HG3	2.18	0.43
1:C:17:ALA:HA	1:C:19:TRP:CZ3	2.53	0.43
1:D:320:VAL:HG12	1:D:320:VAL:O	2.17	0.43
1:D:397:VAL:O	1:D:397:VAL:HG13	2.19	0.43
1:E:17:ALA:O	1:E:20:THR:OG1	2.21	0.43
1:E:32:ASP:O	1:E:35:PHE:CD2	2.71	0.43
1:F:467:ILE:HG22	1:F:468:VAL:H	1.83	0.43
1:G:44:TRP:CG	1:G:45:LEU:N	2.86	0.43
1:H:434:THR:HG22	1:H:520:VAL:HG21	1.99	0.43
1:I:24:GLU:HG3	1:I:24:GLU:O	2.18	0.43
1:J:418:LEU:HA	1:K:66:LYS:NZ	2.33	0.43
1:L:132:TYR:CG	1:L:133:GLU:N	2.87	0.43
1:L:353:PRO:HA	1:L:373:LEU:HB2	2.00	0.43
1:C:309:PHE:CE2	1:C:314:GLU:HA	2.53	0.43
1:C:337:ASN:O	1:C:341:VAL:HG22	2.19	0.43
1:C:403:TYR:CE1	1:D:402:ALA:HA	2.54	0.43
1:C:532:ARG:HE	1:C:558:THR:CG2	2.31	0.43
1:C:69:SER:HA	1:C:72:ARG:NH1	2.32	0.43
1:D:183:GLY:HA2	1:D:186:ASP:HB2	2.00	0.43
1:D:414:GLU:O	1:D:417:THR:OG1	2.29	0.43
1:E:303:VAL:HG13	1:E:303:VAL:O	2.18	0.43
1:G:234:ILE:HG23	1:G:235:TYR:HB3	2.00	0.43
1:G:266:ILE:O	1:G:266:ILE:HG23	2.18	0.43
1:G:306:GLU:O	1:G:307:TRP:HD1	2.01	0.43
1:G:444:LEU:HD22	1:G:517:TYR:CE1	2.54	0.43
1:G:474:VAL:HG13	1:G:475:PRO:HD2	2.00	0.43
1:H:273:ARG:HD3	1:H:275:ARG:NE	2.33	0.43
1:I:280:ILE:HD13	1:I:288:LYS:HE2	2.01	0.43
1:I:279:SER:O	1:I:280:ILE:HG12	2.18	0.43
1:J:499:LEU:HD12	1:J:500:ALA:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:63:VAL:O	1:J:66:LYS:HB2	2.18	0.43
1:K:441:ARG:O	1:K:445:GLU:N	2.39	0.43
1:L:451:ASP:OD1	1:L:453:LEU:HG	2.18	0.43
1:B:299:PRO:HA	1:B:443:ASP:OD1	2.18	0.43
1:C:546:THR:HA	1:C:549:TYR:HB2	2.01	0.43
1:D:328:ARG:O	1:D:332:MET:HG2	2.18	0.43
1:D:484:ASP:H	1:D:488:LYS:HE3	1.83	0.43
1:E:40:GLN:HG3	1:E:41:TRP:CD1	2.53	0.43
1:F:488:LYS:HG3	1:F:489:ASP:N	2.34	0.43
1:I:211:TRP:HE3	1:I:212:LEU:HD22	1.84	0.43
1:J:298:ILE:O	1:J:298:ILE:HG23	2.18	0.43
1:J:446:THR:O	1:J:446:THR:HG22	2.19	0.43
1:K:412:VAL:HA	1:K:415:VAL:HB	2.01	0.43
1:L:337:ASN:OD1	1:L:337:ASN:N	2.52	0.43
1:L:405:LEU:O	1:L:409:THR:N	2.39	0.43
1:A:186:ASP:HA	1:A:189:GLU:HG3	1.99	0.43
1:A:353:PRO:CB	1:A:356:ILE:HB	2.47	0.43
1:A:554:LEU:HD21	1:A:581:VAL:HG11	2.01	0.43
1:C:15:PHE:HD2	1:C:281:ILE:HG12	1.84	0.43
1:C:128:LEU:HG	1:C:300:ILE:HD13	2.00	0.43
1:C:478:VAL:O	1:C:479:THR:OG1	2.36	0.43
1:D:34:PHE:HA	1:D:37:ARG:HG2	2.00	0.43
1:E:254:VAL:O	1:E:254:VAL:HG12	2.19	0.43
1:F:355:GLN:O	1:F:356:ILE:HG22	2.19	0.43
1:F:484:ASP:OD1	1:F:488:LYS:HE2	2.19	0.43
1:J:165:MET:O	1:J:167:LYS:HG3	2.18	0.43
1:J:238:PRO:O	1:J:239:VAL:HG22	2.19	0.43
1:J:320:VAL:HB	1:J:321:ARG:HH21	1.83	0.43
1:J:539:LEU:CD2	1:J:540:GLY:H	2.32	0.43
1:L:457:MET:HG2	1:L:459:ARG:NH2	2.34	0.43
1:L:547:PRO:HG2	1:L:548:GLU:HG3	2.00	0.43
1:L:586:THR:OG1	1:L:587:PRO:HD2	2.18	0.43
1:B:217:ILE:HG23	1:B:217:ILE:O	2.18	0.43
1:B:66:LYS:O	1:B:69:SER:HB2	2.19	0.43
1:B:92:ASP:OD1	1:B:93:VAL:N	2.51	0.43
1:C:106:THR:O	1:C:109:ILE:HG12	2.19	0.43
1:C:64:VAL:HG22	1:C:119:ILE:HG21	2.00	0.43
1:E:362:MET:HG3	1:E:371:TYR:CB	2.48	0.43
1:E:375:ASN:OD1	1:E:377:THR:HG23	2.18	0.43
1:F:203:ASN:OD1	1:F:205:ASN:ND2	2.52	0.43
1:H:214:GLN:O	1:H:216:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:265:LYS:C	1:H:266:ILE:HG13	2.39	0.43
1:I:306:GLU:C	1:I:307:TRP:HD1	2.22	0.43
1:J:161:ASN:O	1:J:162:SER:OG	2.28	0.43
1:K:338:ALA:HA	1:K:341:VAL:HG22	2.01	0.43
1:K:81:ARG:HG2	1:K:519:ASP:HB3	2.00	0.43
1:K:435:VAL:HG23	1:L:108:LYS:HB2	1.99	0.43
1:K:345:PRO:HB2	1:L:371:TYR:CE2	2.54	0.43
1:L:61:ARG:O	1:L:65:ARG:HG2	2.19	0.43
1:A:281:ILE:HG23	1:A:281:ILE:O	2.19	0.43
1:C:128:LEU:HB2	1:C:146:ARG:CG	2.49	0.43
1:D:339:ASP:O	1:D:343:ARG:HB3	2.17	0.43
1:D:448:VAL:HG13	1:D:448:VAL:O	2.19	0.43
1:D:548:GLU:O	1:D:552:LEU:HG	2.19	0.43
1:D:582:LYS:HG3	1:D:583:LYS:N	2.33	0.43
1:D:98:TYR:CZ	1:D:444:LEU:HG	2.53	0.43
1:E:297:HIS:O	1:E:298:ILE:HD13	2.19	0.43
1:F:19:TRP:O	1:F:22:SER:OG	2.22	0.43
1:F:317:GLU:HB3	1:F:321:ARG:HD3	2.01	0.43
1:H:47:GLN:HA	1:I:53:TYR:OH	2.18	0.43
1:I:225:VAL:CG2	1:I:278:LYS:HD2	2.48	0.43
1:I:296:GLU:O	1:I:296:GLU:HG3	2.19	0.43
1:I:354:GLU:HB2	1:I:373:LEU:CD2	2.49	0.43
1:J:9:GLU:N	1:J:9:GLU:OE1	2.52	0.43
1:J:392:TYR:CE2	1:K:349:PRO:HB3	2.54	0.43
1:K:591:GLN:HG2	1:K:592:TRP:H	1.83	0.43
1:A:102:MET:HA	1:A:108:LYS:HD3	2.00	0.43
1:A:339:ASP:HA	1:A:342:ALA:HB3	2.01	0.43
1:B:205:ASN:OD1	1:B:211:TRP:NE1	2.36	0.43
1:C:109:ILE:O	1:C:113:ILE:HG12	2.19	0.43
1:C:280:ILE:HG23	1:C:281:ILE:N	2.34	0.43
1:C:321:ARG:NH1	1:D:41:TRP:HE1	2.16	0.43
1:D:512:GLY:H	1:D:514:TYR:HD2	1.65	0.43
1:D:68:VAL:O	1:D:72:ARG:HB3	2.19	0.43
1:E:119:ILE:HG22	1:E:120:GLU:H	1.83	0.43
1:I:207:TRP:CD1	1:I:208:VAL:HG23	2.53	0.43
1:I:246:TYR:CG	1:I:246:TYR:O	2.72	0.43
1:I:541:LYS:HD3	1:J:532:ARG:HH22	1.84	0.43
1:J:534:GLU:O	1:J:536:LEU:N	2.52	0.43
1:K:266:ILE:HG23	1:K:266:ILE:O	2.18	0.43
1:K:76:ILE:O	1:K:76:ILE:HG23	2.19	0.43
1:A:391:TYR:CE2	1:B:349:PRO:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:GLU:HG2	1:B:296:GLU:O	2.19	0.43
1:C:171:ARG:HG3	1:C:227:GLU:H	1.84	0.43
1:C:93:VAL:HG12	1:C:93:VAL:O	2.19	0.43
1:D:235:TYR:HD2	1:D:258:LEU:H	1.67	0.43
1:E:274:ARG:O	1:E:274:ARG:HG3	2.19	0.43
1:F:322:LEU:HD13	1:F:412:VAL:O	2.19	0.43
1:F:468:VAL:O	1:F:471:ILE:HD12	2.18	0.43
1:F:553:LEU:HD23	1:F:573:ASN:ND2	2.34	0.43
1:G:127:ARG:H	1:G:146:ARG:HH22	1.67	0.43
1:G:331:ASN:O	1:G:334:MET:HB2	2.19	0.43
1:H:387:GLN:HG3	1:H:389:LEU:HD13	2.01	0.43
1:I:348:LYS:O	1:I:348:LYS:HG3	2.19	0.43
1:I:576:LEU:HG	1:I:581:VAL:HG12	2.01	0.43
1:J:116:ARG:NH2	1:J:120:GLU:OE2	2.47	0.43
1:J:169:ASP:C	1:J:171:ARG:H	2.22	0.43
1:J:400:ALA:HA	1:J:403:TYR:CZ	2.54	0.43
1:L:126:TRP:HA	1:L:148:PRO:HA	2.00	0.43
1:L:187:PHE:CE2	1:L:219:ILE:HG21	2.54	0.43
1:L:527:MET:CE	1:L:528:LYS:H	2.32	0.43
1:A:496:VAL:HG13	1:A:497:VAL:N	2.34	0.42
1:A:532:ARG:HH22	1:A:558:THR:HG1	1.63	0.42
1:B:32:ASP:OD2	1:B:154:SER:HB3	2.19	0.42
1:C:156:VAL:HG13	1:C:158:TRP:CE2	2.54	0.42
1:C:34:PHE:HZ	1:C:45:LEU:HD21	1.83	0.42
1:F:233:PHE:CE2	1:F:271:ILE:HD12	2.54	0.42
1:F:35:PHE:HB3	1:F:120:GLU:O	2.19	0.42
1:F:40:GLN:HB3	1:F:41:TRP:CE3	2.54	0.42
1:F:575:GLN:HG3	1:F:576:LEU:H	1.84	0.42
1:H:80:TYR:CD1	1:H:80:TYR:O	2.72	0.42
1:I:255:ILE:HG22	1:I:256:ASP:H	1.84	0.42
1:I:51:LEU:HG	1:I:52:GLN:H	1.83	0.42
1:K:187:PHE:HB2	1:K:190:LYS:HB2	2.00	0.42
1:K:337:ASN:HA	1:K:340:ILE:HG22	2.00	0.42
1:L:67:LEU:HD21	1:L:416:ALA:O	2.19	0.42
1:A:179:MET:N	1:A:218:GLN:OE1	2.36	0.42
1:A:296:GLU:OE1	1:A:450:GLN:HB3	2.19	0.42
1:B:240:THR:O	1:B:240:THR:HG22	2.18	0.42
1:C:559:LEU:O	1:C:560:LEU:HD12	2.19	0.42
1:F:54:ARG:NH2	1:F:331:ASN:O	2.49	0.42
1:H:106:THR:OG1	1:H:145:ARG:NH2	2.35	0.42
1:H:324:LYS:O	1:H:327:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:277:TYR:CZ	1:I:279:SER:HB2	2.54	0.42
1:I:286:VAL:HG23	1:I:288:LYS:HD3	2.01	0.42
1:I:447:TYR:CD1	1:I:447:TYR:O	2.72	0.42
1:I:589:GLU:OE1	1:I:589:GLU:N	2.39	0.42
1:J:185:GLU:O	1:J:185:GLU:HG2	2.19	0.42
1:J:417:THR:O	1:J:418:LEU:HD12	2.18	0.42
1:K:306:GLU:HG3	1:K:316:TYR:OH	2.19	0.42
1:L:31:ASN:HA	1:L:34:PHE:HB2	2.01	0.42
1:A:339:ASP:OD1	1:A:343:ARG:NH1	2.52	0.42
1:A:397:VAL:HG13	1:A:397:VAL:O	2.19	0.42
1:B:126:TRP:CZ3	1:B:128:LEU:HB2	2.54	0.42
1:B:160:SER:HB2	1:B:171:ARG:HE	1.83	0.42
1:C:539:LEU:HD23	1:C:540:GLY:N	2.34	0.42
1:C:65:ARG:NH1	1:C:65:ARG:O	2.45	0.42
1:D:33:LEU:O	1:D:37:ARG:HG2	2.18	0.42
1:D:401:ASN:ND2	1:D:401:ASN:O	2.53	0.42
1:D:60:VAL:HG12	1:D:60:VAL:O	2.18	0.42
1:H:517:TYR:CD1	1:I:103:ARG:HD3	2.55	0.42
1:I:173:CYS:HA	1:I:225:VAL:HG12	2.00	0.42
1:I:392:TYR:CG	1:I:393:GLU:N	2.87	0.42
1:I:74:ASN:O	1:I:76:ILE:HD12	2.19	0.42
1:J:548:GLU:O	1:J:548:GLU:HG2	2.19	0.42
1:L:98:TYR:HE1	1:L:447:TYR:CG	2.38	0.42
1:A:169:ASP:OD1	1:A:170:ALA:N	2.49	0.42
1:A:240:THR:O	1:A:240:THR:HG22	2.20	0.42
1:A:350:PHE:HA	1:A:353:PRO:HD2	2.02	0.42
1:A:369:TYR:HB2	1:A:370:PRO:HD3	2.00	0.42
1:B:280:ILE:HG13	1:B:281:ILE:N	2.32	0.42
1:B:354:GLU:O	1:B:354:GLU:HG3	2.19	0.42
1:B:527:MET:CG	1:B:528:LYS:H	2.30	0.42
1:B:583:LYS:HE2	1:C:563:LYS:HD2	2.00	0.42
1:B:583:LYS:N	1:C:564:GLY:HA3	2.35	0.42
1:D:98:TYR:HA	1:D:101:ASP:OD1	2.19	0.42
1:D:211:TRP:HE1	1:D:213:THR:C	2.23	0.42
1:E:506:VAL:HG21	1:E:510:ILE:HG21	2.01	0.42
1:E:567:MET:HG3	1:E:570:ASP:HB2	2.00	0.42
1:G:347:LYS:HG2	1:G:393:GLU:HG3	2.00	0.42
1:G:309:PHE:HB3	1:H:150:HIS:NE2	2.35	0.42
1:H:279:SER:O	1:H:280:ILE:C	2.56	0.42
1:H:81:ARG:HD3	1:H:517:TYR:HB2	2.02	0.42
1:J:586:THR:N	1:J:587:PRO:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:171:ARG:NE	1:K:226:VAL:H	2.17	0.42
1:K:304:PHE:CZ	1:K:307:TRP:HB2	2.54	0.42
1:K:532:ARG:HG3	1:K:541:LYS:HG3	2.01	0.42
1:B:35:PHE:CZ	1:B:317:GLU:HG3	2.54	0.42
1:B:544:GLN:HA	1:B:548:GLU:OE1	2.19	0.42
1:C:463:ILE:HG22	1:C:463:ILE:O	2.18	0.42
1:D:348:LYS:HA	1:D:348:LYS:HD3	1.74	0.42
1:C:403:TYR:OH	1:D:401:ASN:HB3	2.20	0.42
1:E:100:THR:HA	1:E:102:MET:HG2	2.01	0.42
1:E:297:HIS:CE1	1:E:451:ASP:H	2.37	0.42
1:E:463:ILE:O	1:E:463:ILE:HG22	2.19	0.42
1:E:518:THR:OG1	1:E:520:VAL:HG23	2.19	0.42
1:H:310:VAL:O	1:H:311:GLU:HB2	2.20	0.42
1:H:32:ASP:O	1:H:34:PHE:N	2.53	0.42
1:I:464:TYR:HE1	1:I:465:GLN:HE21	1.68	0.42
1:J:165:MET:HB3	1:J:307:TRP:CH2	2.54	0.42
1:K:116:ARG:O	1:K:120:GLU:HB2	2.19	0.42
1:K:153:CYS:SG	1:K:154:SER:N	2.90	0.42
1:A:11:ILE:O	1:A:11:ILE:HG22	2.19	0.42
1:A:212:LEU:O	1:A:214:GLN:HG3	2.19	0.42
1:D:164:LEU:HG	1:D:166:ASP:O	2.20	0.42
1:E:340:ILE:O	1:E:344:THR:HG23	2.19	0.42
1:H:127:ARG:NH2	1:H:149:ILE:HD11	2.33	0.42
1:H:297:HIS:O	1:H:298:ILE:HG13	2.20	0.42
1:L:162:SER:O	1:L:163:LYS:HB2	2.20	0.42
1:L:441:ARG:HG3	1:L:444:LEU:HB3	2.02	0.42
1:C:254:VAL:HG12	1:C:254:VAL:O	2.19	0.42
1:D:239:VAL:HG13	1:D:240:THR:N	2.35	0.42
1:D:275:ARG:HH21	1:D:290:LYS:HD3	1.84	0.42
1:E:535:ILE:HG13	1:E:536:LEU:H	1.84	0.42
1:F:43:ASP:HB2	1:F:328:ARG:HH22	1.85	0.42
1:G:476:ARG:HG2	1:G:477:ASN:H	1.83	0.42
1:I:306:GLU:O	1:I:307:TRP:HD1	2.03	0.42
1:I:370:PRO:HB2	1:I:372:TYR:CD2	2.55	0.42
1:I:574:LYS:O	1:I:577:ILE:HG23	2.20	0.42
1:K:177:HIS:O	1:K:178:SER:OG	2.26	0.42
1:K:184:TRP:HB3	1:K:187:PHE:CZ	2.55	0.42
1:K:87:ARG:HB2	1:K:88:PRO:HD2	2.02	0.42
1:L:571:TYR:CG	1:L:571:TYR:O	2.73	0.42
1:A:264:ILE:O	1:A:266:ILE:HD12	2.20	0.42
1:A:346:LYS:HG3	1:B:369:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:TRP:N	1:A:353:PRO:CD	2.82	0.42
1:A:503:GLU:HG2	1:A:504:LYS:O	2.19	0.42
1:B:296:GLU:O	1:B:297:HIS:ND1	2.53	0.42
1:C:351:PHE:HB3	1:C:352:TRP:CE3	2.55	0.42
1:C:582:LYS:HG2	1:D:566:GLU:HB2	2.01	0.42
1:D:188:ALA:C	1:D:190:LYS:H	2.22	0.42
1:D:325:ASP:OD1	1:E:53:TYR:OH	2.34	0.42
1:D:461:GLY:C	1:D:463:ILE:H	2.22	0.42
1:E:132:TYR:OH	1:E:137:PRO:HG2	2.20	0.42
1:E:517:TYR:CD2	1:E:518:THR:HG22	2.55	0.42
1:F:350:PHE:HB2	1:F:353:PRO:HG2	2.01	0.42
1:F:356:ILE:HG23	1:F:357:ALA:N	2.34	0.42
1:G:348:LYS:HE2	1:G:350:PHE:HB2	2.01	0.42
1:G:430:VAL:HG12	1:G:431:ALA:N	2.35	0.42
1:H:356:ILE:HG12	1:H:357:ALA:N	2.33	0.42
1:H:471:ILE:HD13	1:H:496:VAL:HA	2.01	0.42
1:J:126:TRP:NE1	1:J:146:ARG:HB2	2.35	0.42
1:J:170:ALA:O	1:J:171:ARG:HB2	2.20	0.42
1:J:345:PRO:HB3	1:K:371:TYR:OH	2.20	0.42
1:K:324:LYS:HD3	1:L:53:TYR:OH	2.20	0.42
1:A:111:VAL:O	1:A:115:VAL:HG13	2.19	0.42
1:A:28:GLU:OE2	1:A:31:ASN:ND2	2.52	0.42
1:A:329:LEU:HD12	1:A:330:ARG:N	2.35	0.42
1:C:352:TRP:CD1	1:C:352:TRP:O	2.73	0.42
1:C:408:ALA:O	1:C:412:VAL:HG23	2.20	0.42
1:D:463:ILE:O	1:D:463:ILE:HG22	2.20	0.42
1:E:462:GLU:C	1:E:463:ILE:HG13	2.40	0.42
1:F:61:ARG:O	1:F:64:VAL:HG12	2.20	0.42
1:G:31:ASN:O	1:G:34:PHE:HD2	2.03	0.42
1:H:109:ILE:O	1:H:111:VAL:N	2.53	0.42
1:H:282:THR:HG22	1:H:283:CYS:N	2.35	0.42
1:I:111:VAL:O	1:I:115:VAL:HG23	2.20	0.42
1:I:387:GLN:HB3	1:I:389:LEU:HD13	2.01	0.42
1:I:345:PRO:HB3	1:I:392:TYR:CZ	2.54	0.42
1:K:324:LYS:HG3	1:L:56:GLN:O	2.19	0.42
1:A:128:LEU:O	1:A:129:VAL:C	2.58	0.42
1:B:453:LEU:H	1:B:453:LEU:CD1	2.33	0.42
1:B:452:ASN:C	1:B:459:ARG:HH12	2.22	0.42
1:B:43:ASP:HB3	1:B:47:GLN:HE22	1.84	0.42
1:C:378:ASP:HB2	1:C:381:SER:HB3	2.02	0.42
1:C:441:ARG:C	1:C:443:ASP:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ILE:O	1:D:109:ILE:HG22	2.19	0.42
1:D:12:LEU:HG	1:D:15:PHE:HB3	2.00	0.42
1:D:567:MET:HG2	1:D:568:MET:N	2.33	0.42
1:E:183:GLY:O	1:E:186:ASP:HB2	2.20	0.42
1:E:192:ASP:OD1	1:E:193:LEU:N	2.52	0.42
1:E:506:VAL:HG23	1:E:508:ASN:H	1.83	0.42
1:D:319:VAL:C	1:E:61:ARG:HH12	2.17	0.42
1:G:156:VAL:HG13	1:G:176:ILE:HD12	2.02	0.42
1:K:66:LYS:O	1:K:70:GLU:N	2.52	0.42
1:L:527:MET:HG3	1:L:528:LYS:N	2.35	0.42
1:L:558:THR:HG23	1:L:559:LEU:N	2.34	0.42
1:B:435:VAL:O	1:B:438:LEU:HG	2.20	0.41
1:C:444:LEU:HD21	1:D:105:ASN:HD21	1.84	0.41
1:C:451:ASP:OD1	1:C:452:ASN:N	2.53	0.41
1:C:558:THR:HG22	1:C:559:LEU:N	2.35	0.41
1:C:76:ILE:O	1:C:76:ILE:HG22	2.19	0.41
1:E:306:GLU:C	1:E:307:TRP:HD1	2.24	0.41
1:G:107:ALA:HB1	1:G:145:ARG:O	2.20	0.41
1:H:104:HIS:CE1	1:H:105:ASN:HD22	2.38	0.41
1:H:249:ARG:HH11	1:H:252:LYS:C	2.23	0.41
1:H:332:MET:O	1:H:335:SER:HB3	2.20	0.41
1:H:63:VAL:HG22	1:H:415:VAL:HG21	2.01	0.41
1:I:451:ASP:CG	1:I:506:VAL:H	2.23	0.41
1:K:107:ALA:HB2	1:K:146:ARG:O	2.20	0.41
1:K:551:LEU:O	1:K:555:GLN:HB2	2.20	0.41
1:L:164:LEU:H	1:L:171:ARG:HH12	1.66	0.41
1:L:276:VAL:CG2	1:L:277:TYR:HD2	2.33	0.41
1:L:311:GLU:HG2	1:L:312:ASP:N	2.35	0.41
1:A:77:ASP:OD2	1:A:525:GLN:NE2	2.53	0.41
1:B:255:ILE:O	1:B:255:ILE:HG22	2.21	0.41
1:B:353:PRO:HA	1:B:374:LEU:HG	2.01	0.41
1:B:541:LYS:HD3	1:C:534:GLU:CD	2.41	0.41
1:D:172:HIS:CE1	1:D:303:VAL:HB	2.55	0.41
1:E:165:MET:HB2	1:E:304:PHE:HA	2.03	0.41
1:G:230:GLU:HG2	1:G:248:LYS:HG2	2.02	0.41
1:I:410:SER:HA	1:I:413:LYS:HG2	2.02	0.41
1:I:447:TYR:HB2	1:I:451:ASP:HA	2.01	0.41
1:I:538:LEU:C	1:I:539:LEU:HD12	2.40	0.41
1:J:280:ILE:HG23	1:J:281:ILE:N	2.34	0.41
1:A:376:ARG:HD2	1:L:384:LEU:HD21	2.02	0.41
1:A:109:ILE:HG13	1:A:112:ASN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:HG12	1:A:324:LYS:HD2	2.02	0.41
1:A:68:VAL:HA	1:A:71:MET:HG2	2.01	0.41
1:C:226:VAL:O	1:C:226:VAL:HG13	2.19	0.41
1:C:341:VAL:HG23	1:C:342:ALA:H	1.85	0.41
1:C:343:ARG:O	1:C:345:PRO:HD3	2.20	0.41
1:C:532:ARG:HH21	1:C:558:THR:HA	1.84	0.41
1:D:345:PRO:HB3	1:D:348:LYS:CE	2.50	0.41
1:E:242:GLU:N	1:E:243:PRO:HD3	2.35	0.41
1:E:282:THR:HG21	1:E:286:VAL:HG13	2.03	0.41
1:E:297:HIS:HB3	1:E:450:GLN:HG3	2.01	0.41
1:E:368:ASP:CG	1:E:369:TYR:H	2.23	0.41
1:F:209:PHE:N	1:F:210:PRO:HD3	2.36	0.41
1:F:442:ALA:O	1:F:446:THR:HG23	2.20	0.41
1:H:452:ASN:N	1:H:452:ASN:OD1	2.53	0.41
1:I:581:VAL:HG23	1:I:583:LYS:N	2.34	0.41
1:J:266:ILE:HG23	1:J:266:ILE:O	2.20	0.41
1:J:324:LYS:HB2	1:K:56:GLN:OE1	2.20	0.41
1:J:459:ARG:CZ	1:J:504:LYS:HA	2.50	0.41
1:A:128:LEU:O	1:A:130:THR:N	2.53	0.41
1:A:511:ARG:HE	1:B:136:SER:HB3	1.85	0.41
1:B:20:THR:HA	1:B:23:ASP:HB3	2.02	0.41
1:B:392:TYR:O	1:B:393:GLU:HG3	2.20	0.41
1:B:66:LYS:N	1:B:66:LYS:HD2	2.35	0.41
1:C:139:SER:O	1:C:142:GLN:NE2	2.51	0.41
1:C:124:GLY:HA3	1:C:152:ALA:HB3	2.01	0.41
1:C:118:GLN:OE1	1:C:432:PHE:HB3	2.21	0.41
1:C:132:TYR:CE1	1:C:455:THR:HG23	2.55	0.41
1:C:524:PHE:HB2	1:C:530:GLN:HB2	2.02	0.41
1:E:580:GLY:HA3	1:F:571:TYR:CE1	2.54	0.41
1:F:289:ASP:OD1	1:F:290:LYS:N	2.53	0.41
1:F:32:ASP:HA	1:F:35:PHE:HB2	2.03	0.41
1:G:156:VAL:HG12	1:G:158:TRP:CE3	2.55	0.41
1:G:61:ARG:N	1:G:62:PRO:CD	2.82	0.41
1:I:170:ALA:HA	1:I:228:LYS:HE3	2.01	0.41
1:J:98:TYR:OH	1:J:516:CYS:SG	2.76	0.41
1:K:184:TRP:NE1	1:K:195:ALA:HB1	2.35	0.41
1:K:240:THR:O	1:K:240:THR:HG22	2.20	0.41
1:L:322:LEU:HD11	1:L:411:ALA:HB1	2.02	0.41
1:A:155:HIS:CE1	1:A:156:VAL:HG12	2.55	0.41
1:A:193:LEU:C	1:A:195:ALA:H	2.24	0.41
1:B:26:ARG:HB3	1:B:313:LYS:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:THR:HB	1:B:352:TRP:CH2	2.56	0.41
1:C:234:ILE:HG13	1:C:234:ILE:O	2.20	0.41
1:C:356:ILE:HG23	1:C:357:ALA:H	1.85	0.41
1:D:343:ARG:O	1:E:366:ASN:ND2	2.53	0.41
1:D:549:TYR:HA	1:D:552:LEU:HD12	2.02	0.41
1:E:224:GLU:OE1	1:E:226:VAL:N	2.52	0.41
1:G:234:ILE:HG13	1:G:235:TYR:N	2.35	0.41
1:H:441:ARG:HH21	1:H:516:CYS:HB3	1.86	0.41
1:H:481:THR:O	1:H:482:LEU:HD12	2.20	0.41
1:I:86:ALA:O	1:I:88:PRO:HD3	2.19	0.41
1:K:311:GLU:O	1:K:314:GLU:OE2	2.39	0.41
1:K:59:VAL:O	1:K:62:PRO:HD2	2.20	0.41
1:B:508:ASN:O	1:B:510:ILE:HG12	2.20	0.41
1:C:38:VAL:HB	1:C:60:VAL:HB	2.02	0.41
1:C:40:GLN:HG2	1:C:41:TRP:N	2.36	0.41
1:C:432:PHE:HB3	1:C:436:ASN:ND2	2.36	0.41
1:D:211:TRP:NE1	1:D:214:GLN:HG2	2.35	0.41
1:D:471:ILE:HG23	1:D:472:TYR:N	2.36	0.41
1:E:234:ILE:HG21	1:E:245:SER:O	2.20	0.41
1:F:222:PHE:HD2	1:F:225:VAL:HG22	1.85	0.41
1:G:16:ASP:O	1:G:20:THR:HG23	2.21	0.41
1:G:310:VAL:N	1:G:314:GLU:OE1	2.54	0.41
1:H:15:PHE:HB3	1:H:281:ILE:CG2	2.49	0.41
1:I:106:THR:O	1:I:109:ILE:HG22	2.20	0.41
1:I:279:SER:O	1:I:280:ILE:CG1	2.68	0.41
1:I:144:ILE:HD13	1:I:445:GLU:O	2.21	0.41
1:I:449:PHE:HE1	1:I:511:ARG:NH2	2.19	0.41
1:J:93:VAL:HG12	1:J:94:LEU:HD12	2.02	0.41
1:K:105:ASN:HD21	1:K:107:ALA:HB3	1.85	0.41
1:A:459:ARG:O	1:A:462:GLU:N	2.54	0.41
1:A:550:GLN:O	1:A:553:LEU:HB3	2.20	0.41
1:B:311:GLU:O	1:B:312:ASP:OD1	2.39	0.41
1:B:42:ASP:CG	1:B:43:ASP:H	2.24	0.41
1:C:57:PHE:HB2	1:C:327:GLN:NE2	2.35	0.41
1:E:314:GLU:O	1:E:314:GLU:HG2	2.21	0.41
1:F:73:GLN:HG3	1:F:73:GLN:O	2.21	0.41
1:G:444:LEU:HD22	1:G:517:TYR:CD1	2.55	0.41
1:H:11:ILE:HG23	1:H:277:TYR:HB3	2.02	0.41
1:I:58:ASP:OD2	1:I:61:ARG:NH2	2.53	0.41
1:J:220:ALA:HB3	1:J:222:PHE:HE2	1.85	0.41
1:J:258:LEU:O	1:J:258:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:163:LYS:O	1:J:307:TRP:NE1	2.53	0.41
1:J:83:LYS:HD3	1:K:100:THR:HG22	2.02	0.41
1:K:213:THR:HG23	1:K:213:THR:O	2.19	0.41
1:K:297:HIS:C	1:K:450:GLN:HE21	2.24	0.41
1:K:83:LYS:HG3	1:K:85:GLY:H	1.86	0.41
1:L:126:TRP:CZ2	1:L:146:ARG:HA	2.55	0.41
1:A:541:LYS:HD3	1:A:541:LYS:HA	1.90	0.41
1:A:93:VAL:O	1:A:93:VAL:HG12	2.21	0.41
1:C:128:LEU:HD12	1:C:128:LEU:O	2.20	0.41
1:C:153:CYS:SG	1:C:154:SER:N	2.93	0.41
1:D:114:ALA:O	1:D:117:GLU:HG2	2.20	0.41
1:E:135:GLN:O	1:E:137:PRO:HD3	2.20	0.41
1:E:172:HIS:CE1	1:E:174:THR:O	2.73	0.41
1:E:58:ASP:OD2	1:E:61:ARG:NH2	2.54	0.41
1:F:39:SER:O	1:F:60:VAL:HG11	2.20	0.41
1:F:405:LEU:O	1:F:409:THR:HG23	2.21	0.41
1:G:564:GLY:O	1:G:567:MET:HG3	2.20	0.41
1:G:592:TRP:O	1:G:593:LEU:C	2.59	0.41
1:H:146:ARG:HD3	1:H:300:ILE:HA	2.02	0.41
1:H:227:GLU:OE2	1:H:229:LYS:HB2	2.21	0.41
1:H:258:LEU:O	1:H:261:SER:OG	2.30	0.41
1:H:26:ARG:HH22	1:H:313:LYS:HE3	1.85	0.41
1:H:507:LEU:H	1:H:513:ARG:HE	1.67	0.41
1:I:34:PHE:O	1:I:38:VAL:N	2.48	0.41
1:I:361:HIS:NE2	1:I:366:ASN:HB3	2.35	0.41
1:I:354:GLU:HB2	1:I:373:LEU:HD22	2.02	0.41
1:J:244:VAL:O	1:J:244:VAL:HG13	2.21	0.41
1:A:151:SER:OG	1:L:309:PHE:N	2.47	0.41
1:A:268:GLU:O	1:A:269:ARG:NH1	2.52	0.41
1:B:125:ALA:H	1:B:148:PRO:HB3	1.86	0.41
1:D:40:GLN:HG3	1:D:41:TRP:HE3	1.85	0.41
1:E:454:ALA:HA	1:E:459:ARG:HH12	1.86	0.41
1:E:509:ASP:O	1:E:510:ILE:C	2.60	0.41
1:F:117:GLU:N	1:F:117:GLU:OE1	2.49	0.41
1:G:58:ASP:O	1:G:59:VAL:HG12	2.21	0.41
1:K:430:VAL:HG12	1:K:431:ALA:N	2.34	0.41
1:L:79:LEU:HD12	1:L:79:LEU:O	2.21	0.41
1:A:323:THR:HA	1:A:327:GLN:NE2	2.35	0.41
1:B:565:VAL:HG12	1:B:565:VAL:O	2.21	0.41
1:C:126:TRP:CD1	1:C:128:LEU:HD23	2.56	0.41
1:D:131:ASP:O	1:D:133:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:PHE:CD2	1:D:438:LEU:HD22	2.56	0.41
1:G:135:GLN:O	1:G:136:SER:OG	2.36	0.41
1:G:356:ILE:HG23	1:G:357:ALA:N	2.35	0.41
1:H:337:ASN:O	1:H:340:ILE:HG13	2.21	0.41
1:I:35:PHE:O	1:I:39:SER:OG	2.29	0.41
1:I:468:VAL:HG13	1:I:471:ILE:HD12	2.01	0.41
1:J:394:ASN:N	1:J:394:ASN:OD1	2.54	0.41
1:L:347:LYS:N	1:L:347:LYS:HD2	2.36	0.41
1:A:300:ILE:CG2	1:A:300:ILE:O	2.69	0.41
1:A:441:ARG:HG3	1:A:442:ALA:H	1.86	0.41
1:B:488:LYS:HG2	1:B:489:ASP:N	2.36	0.41
1:C:15:PHE:CD2	1:C:281:ILE:HG12	2.55	0.41
1:F:392:TYR:OH	1:G:351:PHE:O	2.32	0.41
1:H:334:MET:HA	1:H:337:ASN:OD1	2.21	0.41
1:J:12:LEU:HG	1:J:15:PHE:HB3	2.03	0.41
1:J:61:ARG:N	1:J:62:PRO:HD2	2.35	0.41
1:K:321:ARG:HD2	1:K:324:LYS:HB3	2.03	0.41
1:K:87:ARG:HG3	1:K:89:ASP:OD1	2.21	0.41
1:L:197:ASP:OD1	1:L:198:ILE:N	2.43	0.41
1:A:237:ASP:O	1:A:242:GLU:HG3	2.20	0.40
1:A:551:LEU:HD22	1:B:567:MET:HG3	2.03	0.40
1:C:132:TYR:CZ	1:C:454:ALA:HB1	2.56	0.40
1:C:299:PRO:O	1:C:301:VAL:HG23	2.21	0.40
1:E:224:GLU:OE1	1:E:227:GLU:N	2.54	0.40
1:E:480:ILE:HG13	1:E:481:THR:H	1.85	0.40
1:F:526:SER:HB2	1:F:530:GLN:CG	2.50	0.40
1:G:376:ARG:HG2	1:G:376:ARG:O	2.21	0.40
1:H:339:ASP:O	1:H:343:ARG:HG2	2.20	0.40
1:H:371:TYR:CE2	1:H:373:LEU:HD12	2.56	0.40
1:H:541:LYS:HB3	1:I:535:ILE:HG21	2.03	0.40
1:I:565:VAL:O	1:I:565:VAL:HG12	2.21	0.40
1:J:108:LYS:O	1:J:111:VAL:HG22	2.21	0.40
1:L:93:VAL:HG23	1:L:94:LEU:N	2.37	0.40
1:A:528:LYS:HB3	1:A:532:ARG:HB2	2.03	0.40
1:B:441:ARG:NH2	1:C:103:ARG:O	2.54	0.40
1:C:445:GLU:O	1:C:449:PHE:N	2.54	0.40
1:D:566:GLU:N	1:D:566:GLU:OE1	2.54	0.40
1:F:403:TYR:HA	1:F:406:GLU:OE1	2.21	0.40
1:G:336:PHE:CZ	1:G:397:VAL:HG22	2.56	0.40
1:H:155:HIS:O	1:H:157:ILE:HD12	2.21	0.40
1:H:483:GLU:O	1:H:484:ASP:OD1	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:235:TYR:OH	1:I:249:ARG:NH1	2.54	0.40
1:J:420:VAL:O	1:J:426:ASN:ND2	2.48	0.40
1:J:430:VAL:HG13	1:J:432:PHE:H	1.85	0.40
1:J:58:ASP:N	1:J:58:ASP:OD1	2.52	0.40
1:K:272:LYS:O	1:K:272:LYS:HG3	2.21	0.40
1:K:289:ASP:CG	1:K:290:LYS:H	2.24	0.40
1:K:406:GLU:HA	1:K:409:THR:HB	2.03	0.40
1:L:214:GLN:O	1:L:216:THR:HG23	2.21	0.40
1:L:80:TYR:CE2	1:L:98:TYR:HB3	2.56	0.40
1:A:292:LEU:HD21	1:A:295:GLY:H	1.86	0.40
1:A:574:LYS:HB2	1:A:576:LEU:HB3	2.03	0.40
1:B:320:VAL:HG11	1:B:415:VAL:HB	2.02	0.40
1:B:354:GLU:H	1:B:374:LEU:HG	1.85	0.40
1:B:539:LEU:CG	1:B:540:GLY:H	2.34	0.40
1:C:198:ILE:HG22	1:C:198:ILE:O	2.20	0.40
1:D:193:LEU:HD12	1:D:195:ALA:H	1.86	0.40
1:D:296:GLU:OE1	1:D:296:GLU:N	2.54	0.40
1:E:226:VAL:HG23	1:E:227:GLU:H	1.86	0.40
1:F:318:GLY:O	1:F:321:ARG:HG3	2.21	0.40
1:G:280:ILE:HG12	1:G:288:LYS:CD	2.49	0.40
1:G:280:ILE:HG21	1:G:288:LYS:HE2	2.03	0.40
1:H:72:ARG:NH1	1:H:112:ASN:OD1	2.54	0.40
1:H:123:VAL:HG13	1:H:303:VAL:HG23	2.04	0.40
1:H:488:LYS:NZ	1:H:491:GLN:HA	2.37	0.40
1:J:236:GLN:HG3	1:J:247:PHE:CZ	2.57	0.40
1:J:321:ARG:HH11	1:J:327:GLN:HE21	1.67	0.40
1:J:403:TYR:OH	1:K:401:ASN:ND2	2.54	0.40
1:K:264:ILE:HG12	1:K:265:LYS:H	1.86	0.40
1:B:156:VAL:O	1:B:156:VAL:HG13	2.21	0.40
1:C:126:TRP:NE1	1:C:128:LEU:HD23	2.36	0.40
1:C:430:VAL:HG13	1:C:432:PHE:HB2	2.04	0.40
1:C:546:THR:HG23	1:C:547:PRO:HD3	2.03	0.40
1:D:123:VAL:HB	1:D:152:ALA:HB1	2.04	0.40
1:E:78:VAL:HG12	1:E:525:GLN:HA	2.04	0.40
1:F:370:PRO:HG2	1:F:372:TYR:CZ	2.56	0.40
1:G:249:ARG:HD3	1:G:252:LYS:HG2	2.03	0.40
1:G:57:PHE:HB3	1:G:331:ASN:OD1	2.22	0.40
1:H:372:TYR:CG	1:H:373:LEU:N	2.90	0.40
1:I:282:THR:HG22	1:I:284:THR:H	1.86	0.40
1:I:301:VAL:HG12	1:I:302:PRO:O	2.22	0.40
1:J:63:VAL:CG2	1:J:320:VAL:HG11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:80:TYR:CE2	1:K:82:PRO:HG3	2.56	0.40
1:L:126:TRP:HZ2	1:L:146:ARG:HA	1.86	0.40
1:K:248:LYS:HD3	1:L:190:LYS:O	2.22	0.40
1:L:345:PRO:O	1:L:346:LYS:HB2	2.21	0.40
1:A:520:VAL:HG11	1:B:105:ASN:ND2	2.36	0.40
1:B:550:GLN:O	1:B:553:LEU:HD13	2.21	0.40
1:B:80:TYR:CE2	1:C:563:LYS:HE3	2.57	0.40
1:D:42:ASP:N	1:D:42:ASP:OD1	2.55	0.40
1:D:582:LYS:HG3	1:D:583:LYS:HG2	2.04	0.40
1:D:587:PRO:HB2	1:D:588:GLU:OE1	2.21	0.40
1:F:306:GLU:HG2	1:F:435:VAL:HG21	2.04	0.40
1:F:59:VAL:HG13	1:F:59:VAL:O	2.22	0.40
1:H:392:TYR:HB2	1:I:349:PRO:HB3	2.03	0.40
1:H:577:ILE:HG13	1:H:578:GLN:N	2.36	0.40
1:I:14:ARG:HH22	1:I:225:VAL:CG2	2.35	0.40
1:I:249:ARG:NH2	1:I:251:ILE:HB	2.37	0.40
1:J:124:GLY:O	1:J:303:VAL:N	2.54	0.40
1:J:60:VAL:HG12	1:J:60:VAL:O	2.21	0.40
1:K:246:TYR:CE2	1:K:272:LYS:HD2	2.57	0.40
1:K:352:TRP:N	1:K:353:PRO:CD	2.84	0.40
1:K:78:VAL:HG12	1:K:524:PHE:O	2.22	0.40
1:L:198:ILE:O	1:L:198:ILE:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	583/610 (96%)	461 (79%)	115 (20%)	7 (1%)	13 42
1	B	583/610 (96%)	461 (79%)	112 (19%)	10 (2%)	9 35
1	C	583/610 (96%)	442 (76%)	130 (22%)	11 (2%)	8 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	583/610 (96%)	451 (77%)	123 (21%)	9 (2%)	10	38
1	E	583/610 (96%)	454 (78%)	120 (21%)	9 (2%)	10	38
1	F	583/610 (96%)	448 (77%)	129 (22%)	6 (1%)	15	46
1	G	583/610 (96%)	438 (75%)	135 (23%)	10 (2%)	9	35
1	H	583/610 (96%)	440 (76%)	134 (23%)	9 (2%)	10	38
1	I	583/610 (96%)	436 (75%)	137 (24%)	10 (2%)	9	35
1	J	583/610 (96%)	443 (76%)	132 (23%)	8 (1%)	11	38
1	K	583/610 (96%)	455 (78%)	121 (21%)	7 (1%)	13	42
1	L	583/610 (96%)	450 (77%)	125 (21%)	8 (1%)	11	38
All	All	6996/7320 (96%)	5379 (77%)	1513 (22%)	104 (2%)	10	38

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	VAL
1	B	226	VAL
1	B	244	VAL
1	B	282	THR
1	C	281	ILE
1	D	463	ILE
1	E	463	ILE
1	F	76	ILE
1	I	506	VAL
1	J	463	ILE
1	J	506	VAL
1	L	244	VAL
1	L	463	ILE
1	C	370	PRO
1	C	506	VAL
1	E	59	VAL
1	E	300	ILE
1	E	506	VAL
1	G	234	ILE
1	I	59	VAL
1	I	210	PRO
1	I	581	VAL
1	J	170	ALA
1	K	280	ILE
1	B	506	VAL

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Mol	Chain	Res	Type
1	D	356	ILE
1	F	467	ILE
1	H	254	VAL
1	H	356	ILE
1	I	496	VAL
1	K	535	ILE
1	A	144	ILE
1	A	226	VAL
1	A	353	PRO
1	B	356	ILE
1	B	463	ILE
1	C	356	ILE
1	C	535	ILE
1	D	190	LYS
1	D	506	VAL
1	E	119	ILE
1	E	425	VAL
1	F	356	ILE
1	G	338	ALA
1	G	356	ILE
1	G	506	VAL
1	G	535	ILE
1	H	577	ILE
1	J	280	ILE
1	J	577	ILE
1	K	356	ILE
1	L	226	VAL
1	L	280	ILE
1	L	281	ILE
1	L	356	ILE
1	L	506	VAL
1	B	140	ASN
1	G	370	PRO
1	G	388	PRO
1	H	418	LEU
1	I	57	PHE
1	I	353	PRO
1	A	463	ILE
1	C	129	VAL
1	F	178	SER
1	F	217	ILE
1	K	129	VAL

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Mol	Chain	Res	Type
1	K	353	PRO
1	D	226	VAL
1	D	244	VAL
1	F	463	ILE
1	H	76	ILE
1	J	76	ILE
1	J	244	VAL
1	J	369	TYR
1	K	76	ILE
1	L	353	PRO
1	B	76	ILE
1	C	76	ILE
1	C	234	ILE
1	C	353	PRO
1	D	303	VAL
1	E	76	ILE
1	I	76	ILE
1	I	244	VAL
1	K	234	ILE
1	A	217	ILE
1	C	276	VAL
1	D	471	ILE
1	H	234	ILE
1	A	480	ILE
1	C	251	ILE
1	D	123	VAL
1	E	217	ILE
1	E	587	PRO
1	G	217	ILE
1	G	497	VAL
1	H	217	ILE
1	H	266	ILE
1	H	280	ILE
1	I	266	ILE
1	A	76	ILE
1	B	217	ILE
1	G	463	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	512/536 (96%)	512 (100%)	0	100 100
1	B	508/536 (95%)	506 (100%)	2 (0%)	91 95
1	C	508/536 (95%)	508 (100%)	0	100 100
1	D	512/536 (96%)	511 (100%)	1 (0%)	93 97
1	E	511/536 (95%)	511 (100%)	0	100 100
1	F	508/536 (95%)	508 (100%)	0	100 100
1	G	507/536 (95%)	505 (100%)	2 (0%)	91 95
1	H	508/536 (95%)	508 (100%)	0	100 100
1	I	508/536 (95%)	506 (100%)	2 (0%)	91 95
1	J	508/536 (95%)	506 (100%)	2 (0%)	91 95
1	K	510/536 (95%)	510 (100%)	0	100 100
1	L	508/536 (95%)	508 (100%)	0	100 100
All	All	6108/6432 (95%)	6099 (100%)	9 (0%)	93 97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	193	LEU
1	B	453	LEU
1	D	507	LEU
1	G	350	PHE
1	G	351	PHE
1	I	374	LEU
1	I	447	TYR
1	J	324	LYS
1	J	539	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	525	GLN
1	C	104	HIS
1	D	118	GLN

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Mol	Chain	Res	Type
1	D	142	GLN
1	D	401	ASN
1	D	436	ASN
1	F	205	ASN
1	F	218	GLN
1	G	236	GLN
1	G	366	ASN
1	G	437	GLN
1	I	401	ASN
1	I	437	GLN
1	K	450	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	585/610 (95%)	0.36	42 (7%) 15 15	16, 65, 94, 113	0
1	B	585/610 (95%)	0.28	35 (5%) 21 21	19, 62, 89, 109	0
1	C	585/610 (95%)	0.36	54 (9%) 9 9	19, 61, 91, 130	0
1	D	585/610 (95%)	0.56	62 (10%) 6 6	21, 66, 97, 184	0
1	E	585/610 (95%)	0.41	51 (8%) 10 10	19, 63, 98, 205	0
1	F	585/610 (95%)	0.36	42 (7%) 15 15	22, 60, 94, 142	0
1	G	585/610 (95%)	0.40	57 (9%) 7 8	18, 59, 92, 136	0
1	H	585/610 (95%)	0.38	53 (9%) 9 9	20, 62, 93, 117	0
1	I	585/610 (95%)	0.39	45 (7%) 13 12	19, 66, 99, 192	0
1	J	585/610 (95%)	0.45	66 (11%) 5 5	21, 65, 97, 142	0
1	K	585/610 (95%)	0.39	54 (9%) 9 9	27, 67, 100, 132	0
1	L	585/610 (95%)	0.40	54 (9%) 9 9	21, 64, 102, 156	0
All	All	7020/7320 (95%)	0.39	615 (8%) 10 10	16, 63, 96, 205	0

All (615) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	238	PRO	11.8
1	E	232	ALA	11.4
1	D	558	THR	10.9
1	L	516	CYS	9.0
1	D	516	CYS	8.5
1	E	237	ASP	8.3
1	J	86	ALA	8.1
1	L	212	LEU	7.8
1	F	302	PRO	7.8
1	K	436	ASN	7.7
1	F	305	GLY	7.6

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Mol	Chain	Res	Type	RSRZ
1	B	245	SER	7.5
1	F	460	ASP	7.5
1	C	574	LYS	7.5
1	G	13	SER	7.3
1	J	531	ASN	7.3
1	E	231	THR	7.2
1	I	84	ASP	7.0
1	L	161	ASN	7.0
1	F	304	PHE	6.9
1	K	426	ASN	6.9
1	B	160	SER	6.8
1	E	516	CYS	6.7
1	D	195	ALA	6.6
1	K	404	MET	6.5
1	C	231	THR	6.5
1	H	572	ALA	6.5
1	K	435	VAL	6.3
1	D	460	ASP	6.3
1	G	83	LYS	5.9
1	I	125	ALA	5.9
1	G	469	ASN	5.8
1	C	125	ALA	5.7
1	J	46	SER	5.6
1	J	443	ASP	5.6
1	K	29	ALA	5.6
1	D	526	SER	5.5
1	D	524	PHE	5.5
1	G	453	LEU	5.5
1	D	502	GLY	5.5
1	B	220	ALA	5.5
1	D	9	GLU	5.5
1	I	437	GLN	5.5
1	A	203	ASN	5.5
1	G	238	PRO	5.5
1	I	564	GLY	5.4
1	G	39	SER	5.4
1	E	318	GLY	5.4
1	G	461	GLY	5.4
1	A	32	ASP	5.4
1	H	22	SER	5.4
1	F	442	ALA	5.3
1	L	205	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
1	E	578	GLN	5.3
1	H	430	VAL	5.3
1	I	231	THR	5.2
1	L	462	GLU	5.2
1	A	447	TYR	5.2
1	C	506	VAL	5.2
1	A	439	ASN	5.1
1	F	50	THR	5.1
1	K	425	VAL	5.1
1	G	558	THR	5.0
1	H	566	GLU	5.0
1	I	565	VAL	5.0
1	A	464	TYR	5.0
1	I	126	TRP	5.0
1	G	175	VAL	5.0
1	H	565	VAL	5.0
1	H	375	ASN	5.0
1	F	267	ALA	5.0
1	H	90	ALA	5.0
1	E	460	ASP	4.9
1	H	125	ALA	4.9
1	D	255	ILE	4.9
1	D	174	THR	4.9
1	L	125	ALA	4.8
1	C	292	LEU	4.8
1	D	206	ASP	4.8
1	D	316	TYR	4.8
1	F	580	GLY	4.8
1	J	461	GLY	4.7
1	G	42	ASP	4.7
1	D	196	ASP	4.7
1	E	32	ASP	4.7
1	H	151	SER	4.7
1	A	364	ASP	4.6
1	D	562	GLY	4.6
1	J	510	ILE	4.6
1	I	483	GLU	4.6
1	J	42	ASP	4.6
1	L	294	ALA	4.6
1	J	174	THR	4.5
1	J	464	TYR	4.5
1	D	426	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	K	153	CYS	4.5
1	A	262	GLY	4.5
1	J	85	GLY	4.5
1	K	361	HIS	4.5
1	D	559	LEU	4.4
1	K	44	TRP	4.4
1	K	428	GLY	4.4
1	K	294	ALA	4.4
1	G	468	VAL	4.4
1	D	220	ALA	4.4
1	B	282	THR	4.4
1	G	123	VAL	4.4
1	J	43	ASP	4.4
1	J	118	GLN	4.4
1	B	243	PRO	4.3
1	D	416	ALA	4.3
1	G	241	GLY	4.3
1	L	168	SER	4.3
1	J	307	TRP	4.3
1	K	36	SER	4.3
1	C	395	PRO	4.3
1	L	149	ILE	4.3
1	G	174	THR	4.3
1	I	85	GLY	4.2
1	G	481	THR	4.2
1	F	377	THR	4.2
1	G	84	ASP	4.2
1	K	28	GLU	4.2
1	G	200	SER	4.2
1	L	206	ASP	4.2
1	D	286	VAL	4.2
1	C	164	LEU	4.1
1	I	455	THR	4.1
1	A	296	GLU	4.1
1	H	85	GLY	4.1
1	E	302	PRO	4.1
1	L	293	ILE	4.1
1	C	259	ALA	4.1
1	A	481	THR	4.1
1	H	176	ILE	4.1
1	D	250	ASP	4.1
1	C	533	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	279	SER	4.0
1	I	369	TYR	4.0
1	F	461	GLY	4.0
1	J	175	VAL	4.0
1	E	30	LYS	4.0
1	E	435	VAL	4.0
1	K	526	SER	4.0
1	H	89	ASP	4.0
1	I	484	ASP	4.0
1	E	29	ALA	4.0
1	A	295	GLY	4.0
1	K	100	THR	4.0
1	G	494	ALA	4.0
1	A	281	ILE	3.9
1	D	18	ASP	3.9
1	H	562	GLY	3.9
1	L	240	THR	3.9
1	G	32	ASP	3.9
1	G	124	GLY	3.9
1	C	172	HIS	3.9
1	I	122	GLY	3.9
1	C	220	ALA	3.9
1	K	337	ASN	3.9
1	G	12	LEU	3.8
1	C	105	ASN	3.8
1	D	282	THR	3.8
1	J	365	GLY	3.8
1	K	154	SER	3.8
1	E	156	VAL	3.8
1	J	495	GLU	3.8
1	E	33	LEU	3.8
1	I	282	THR	3.8
1	H	518	THR	3.7
1	A	461	GLY	3.7
1	F	428	GLY	3.7
1	F	100	THR	3.7
1	A	440	MET	3.7
1	E	461	GLY	3.7
1	D	448	VAL	3.7
1	E	107	ALA	3.7
1	K	481	THR	3.7
1	E	236	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	444	LEU	3.7
1	C	553	LEU	3.7
1	C	566	GLU	3.7
1	A	377	THR	3.6
1	E	437	GLN	3.6
1	C	507	LEU	3.6
1	B	573	ASN	3.6
1	A	46	SER	3.6
1	F	268	GLU	3.6
1	G	173	CYS	3.6
1	G	439	ASN	3.6
1	K	453	LEU	3.6
1	H	205	ASN	3.6
1	D	446	THR	3.6
1	I	442	ALA	3.6
1	C	104	HIS	3.6
1	K	268	GLU	3.6
1	E	370	PRO	3.5
1	G	566	GLU	3.5
1	G	292	LEU	3.5
1	I	138	THR	3.5
1	C	279	SER	3.5
1	L	448	VAL	3.5
1	C	238	PRO	3.5
1	K	590	GLN	3.5
1	B	50	THR	3.5
1	J	12	LEU	3.5
1	F	358	GLY	3.5
1	H	584	PRO	3.5
1	E	255	ILE	3.5
1	K	591	GLN	3.4
1	J	516	CYS	3.4
1	D	104	HIS	3.4
1	F	101	ASP	3.4
1	C	82	PRO	3.4
1	I	103	ARG	3.4
1	J	270	GLN	3.4
1	H	208	VAL	3.4
1	K	291	GLN	3.4
1	I	123	VAL	3.4
1	D	251	ILE	3.4
1	K	32	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	539	LEU	3.4
1	D	17	ALA	3.4
1	L	517	TYR	3.4
1	L	553	LEU	3.4
1	H	29	ALA	3.3
1	J	170	ALA	3.3
1	F	293	ILE	3.3
1	C	529	GLN	3.3
1	L	345	PRO	3.3
1	J	301	VAL	3.3
1	C	177	HIS	3.3
1	H	267	ALA	3.3
1	I	191	TYR	3.3
1	A	570	ASP	3.3
1	J	21	ALA	3.3
1	K	31	ASN	3.3
1	K	527	MET	3.3
1	E	283	CYS	3.3
1	K	427	GLY	3.3
1	G	534	GLU	3.3
1	B	262	GLY	3.3
1	D	287	LEU	3.3
1	B	151	SER	3.2
1	I	220	ALA	3.2
1	E	262	GLY	3.2
1	D	272	LYS	3.2
1	B	267	ALA	3.2
1	H	464	TYR	3.2
1	E	150	HIS	3.2
1	F	12	LEU	3.2
1	L	209	PHE	3.2
1	L	239	VAL	3.2
1	I	280	ILE	3.2
1	E	284	THR	3.2
1	J	530	GLN	3.2
1	H	21	ALA	3.1
1	I	139	SER	3.1
1	D	533	ALA	3.1
1	K	289	ASP	3.1
1	B	95	MET	3.1
1	H	130	THR	3.1
1	K	573	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	232	ALA	3.1
1	J	293	ILE	3.1
1	J	308	GLY	3.1
1	E	301	VAL	3.1
1	K	501	THR	3.1
1	J	318	GLY	3.1
1	L	118	GLN	3.1
1	J	45	LEU	3.1
1	H	377	THR	3.1
1	G	567	MET	3.1
1	C	91	ALA	3.1
1	C	237	ASP	3.0
1	I	124	GLY	3.0
1	B	516	CYS	3.0
1	G	170	ALA	3.0
1	G	22	SER	3.0
1	L	147	GLU	3.0
1	B	51	LEU	3.0
1	H	424	ALA	3.0
1	A	438	LEU	3.0
1	J	155	HIS	3.0
1	I	414	GLU	3.0
1	K	281	ILE	3.0
1	H	226	VAL	3.0
1	H	279	SER	3.0
1	H	291	GLN	3.0
1	D	461	GLY	3.0
1	J	512	GLY	3.0
1	L	285	ALA	3.0
1	K	174	THR	3.0
1	F	485	GLY	3.0
1	E	110	ALA	3.0
1	H	376	ARG	3.0
1	A	106	THR	3.0
1	E	213	THR	3.0
1	J	565	VAL	2.9
1	C	525	GLN	2.9
1	E	463	ILE	2.9
1	I	566	GLU	2.9
1	A	448	VAL	2.9
1	E	279	SER	2.9
1	F	494	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	96	GLY	2.9
1	H	465	GLN	2.9
1	H	561	ASP	2.9
1	D	279	SER	2.9
1	I	485	GLY	2.9
1	C	565	VAL	2.9
1	L	235	TYR	2.9
1	H	275	ARG	2.9
1	A	198	ILE	2.9
1	J	219	ILE	2.9
1	I	338	ALA	2.9
1	G	43	ASP	2.9
1	L	75	PRO	2.9
1	G	36	SER	2.8
1	C	357	ALA	2.8
1	G	360	GLU	2.8
1	D	169	ASP	2.8
1	E	553	LEU	2.8
1	E	580	GLY	2.8
1	E	200	SER	2.8
1	A	582	LYS	2.8
1	F	294	ALA	2.8
1	B	445	GLU	2.8
1	D	231	THR	2.8
1	A	508	ASN	2.8
1	J	562	GLY	2.8
1	G	117	GLU	2.8
1	J	388	PRO	2.8
1	I	39	SER	2.8
1	F	170	ALA	2.8
1	A	126	TRP	2.8
1	B	517	TYR	2.8
1	L	151	SER	2.8
1	I	463	ILE	2.8
1	K	193	LEU	2.8
1	H	580	GLY	2.8
1	J	207	TRP	2.8
1	F	102	MET	2.8
1	G	562	GLY	2.8
1	D	256	ASP	2.8
1	L	194	ASP	2.8
1	E	139	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	566	GLU	2.7
1	G	266	ILE	2.7
1	D	194	ASP	2.7
1	J	459	ARG	2.7
1	J	467	ILE	2.7
1	A	486	SER	2.7
1	L	485	GLY	2.7
1	F	301	VAL	2.7
1	J	286	VAL	2.7
1	J	442	ALA	2.7
1	B	32	ASP	2.7
1	L	116	ARG	2.7
1	H	20	THR	2.7
1	B	442	ALA	2.7
1	D	10	SER	2.6
1	I	50	THR	2.6
1	D	170	ALA	2.6
1	D	193	LEU	2.6
1	H	23	ASP	2.6
1	D	459	ARG	2.6
1	J	287	LEU	2.6
1	K	470	ASP	2.6
1	J	300	ILE	2.6
1	C	564	GLY	2.6
1	J	466	SER	2.6
1	L	477	ASN	2.6
1	C	159	ASP	2.6
1	G	278	LYS	2.6
1	L	188	ALA	2.6
1	I	207	TRP	2.6
1	B	279	SER	2.6
1	C	43	ASP	2.6
1	E	17	ALA	2.6
1	B	501	THR	2.6
1	A	308	GLY	2.6
1	A	463	ILE	2.6
1	K	214	GLN	2.6
1	D	447	TYR	2.6
1	A	225	VAL	2.6
1	H	91	ALA	2.6
1	H	350	PHE	2.6
1	A	208	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	315	VAL	2.6
1	B	106	THR	2.6
1	C	18	ASP	2.5
1	H	43	ASP	2.5
1	G	97	MET	2.5
1	C	361	HIS	2.5
1	D	20	THR	2.5
1	K	488	LYS	2.5
1	C	505	GLN	2.5
1	H	268	GLU	2.5
1	B	122	GLY	2.5
1	H	124	GLY	2.5
1	C	160	SER	2.5
1	H	363	TYR	2.5
1	H	322	LEU	2.5
1	B	263	PHE	2.5
1	C	196	ASP	2.5
1	G	466	SER	2.5
1	J	460	ASP	2.5
1	G	26	ARG	2.5
1	D	445	GLU	2.5
1	H	517	TYR	2.5
1	E	207	TRP	2.5
1	G	222	PHE	2.5
1	A	146	ARG	2.5
1	F	144	ILE	2.5
1	C	254	VAL	2.5
1	L	501	THR	2.5
1	C	124	GLY	2.5
1	J	283	CYS	2.5
1	F	136	SER	2.5
1	H	118	GLN	2.5
1	C	126	TRP	2.5
1	L	41	TRP	2.5
1	C	472	TYR	2.5
1	J	444	LEU	2.5
1	L	112	ASN	2.5
1	L	461	GLY	2.5
1	E	577	ILE	2.5
1	C	394	ASN	2.4
1	A	522	PRO	2.4
1	H	84	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	510	ILE	2.4
1	J	243	PRO	2.4
1	J	25	ALA	2.4
1	A	469	ASN	2.4
1	F	137	PRO	2.4
1	A	180	SER	2.4
1	D	213	THR	2.4
1	D	173	CYS	2.4
1	F	88	PRO	2.4
1	J	253	ASP	2.4
1	D	454	ALA	2.4
1	A	307	TRP	2.4
1	B	232	ALA	2.4
1	L	511	ARG	2.4
1	C	587	PRO	2.4
1	L	436	ASN	2.4
1	F	29	ALA	2.4
1	H	131	ASP	2.4
1	E	198	ILE	2.4
1	B	285	ALA	2.4
1	C	219	ILE	2.4
1	F	378	ASP	2.4
1	H	99	ARG	2.4
1	C	555	GLN	2.4
1	J	39	SER	2.4
1	K	469	ASN	2.4
1	B	21	ALA	2.4
1	K	237	ASP	2.4
1	D	538	LEU	2.4
1	I	242	GLU	2.4
1	J	386	THR	2.4
1	F	145	ARG	2.4
1	F	335	SER	2.4
1	D	259	ALA	2.4
1	L	479	THR	2.4
1	C	253	ASP	2.3
1	G	201	PHE	2.3
1	A	523	SER	2.3
1	K	261	SER	2.3
1	J	514	TYR	2.3
1	F	161	ASN	2.3
1	I	182	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	13	SER	2.3
1	E	45	LEU	2.3
1	B	570	ASP	2.3
1	K	12	LEU	2.3
1	B	383	ASP	2.3
1	A	466	SER	2.3
1	F	465	GLN	2.3
1	J	471	ILE	2.3
1	D	589	GLU	2.3
1	B	264	ILE	2.3
1	L	42	ASP	2.3
1	E	209	PHE	2.3
1	L	279	SER	2.3
1	B	123	VAL	2.3
1	L	427	GLY	2.3
1	J	151	SER	2.3
1	E	280	ILE	2.3
1	A	366	ASN	2.3
1	J	463	ILE	2.3
1	C	567	MET	2.3
1	I	438	LEU	2.3
1	K	440	MET	2.3
1	J	119	ILE	2.3
1	J	387	GLN	2.3
1	L	28	GLU	2.3
1	D	249	ARG	2.3
1	L	554	LEU	2.3
1	B	244	VAL	2.3
1	D	123	VAL	2.3
1	J	232	ALA	2.3
1	J	305	GLY	2.2
1	J	515	GLU	2.2
1	H	454	ALA	2.2
1	H	126	TRP	2.2
1	C	334	MET	2.2
1	E	508	ASN	2.2
1	K	173	CYS	2.2
1	I	557	PHE	2.2
1	L	263	PHE	2.2
1	L	581	VAL	2.2
1	G	533	ALA	2.2
1	D	436	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	89	ASP	2.2
1	I	104	HIS	2.2
1	C	309	PHE	2.2
1	L	146	ARG	2.2
1	I	362	MET	2.2
1	A	188	ALA	2.2
1	A	128	LEU	2.2
1	E	593	LEU	2.2
1	F	307	TRP	2.2
1	G	234	ILE	2.2
1	J	145	ARG	2.2
1	F	241	GLY	2.2
1	D	294	ALA	2.2
1	G	47	GLN	2.2
1	K	390	ALA	2.2
1	A	47	GLN	2.2
1	E	138	THR	2.2
1	L	50	THR	2.2
1	L	81	ARG	2.2
1	L	568	MET	2.2
1	B	554	LEU	2.2
1	K	86	ALA	2.2
1	D	437	GLN	2.2
1	E	199	PRO	2.2
1	G	148	PRO	2.2
1	C	436	ASN	2.2
1	G	240	THR	2.2
1	G	293	ILE	2.2
1	G	472	TYR	2.2
1	B	124	GLY	2.2
1	C	552	LEU	2.1
1	J	242	GLU	2.1
1	J	587	PRO	2.1
1	A	318	GLY	2.1
1	K	516	CYS	2.1
1	C	401	ASN	2.1
1	E	366	ASN	2.1
1	G	248	LYS	2.1
1	K	245	SER	2.1
1	E	289	ASP	2.1
1	E	558	THR	2.1
1	G	446	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	338	ALA	2.1
1	C	532	ARG	2.1
1	I	172	HIS	2.1
1	J	529	GLN	2.1
1	G	523	SER	2.1
1	L	51	LEU	2.1
1	J	364	ASP	2.1
1	D	188	ALA	2.1
1	F	126	TRP	2.1
1	G	306	GLU	2.1
1	H	502	GLY	2.1
1	L	241	GLY	2.1
1	E	330	ARG	2.1
1	I	549	TYR	2.1
1	L	152	ALA	2.1
1	K	344	THR	2.1
1	K	269	ARG	2.1
1	F	403	TYR	2.1
1	G	188	ALA	2.1
1	I	460	ASP	2.1
1	B	150	HIS	2.1
1	K	46	SER	2.1
1	K	548	GLU	2.1
1	H	468	VAL	2.1
1	J	363	TYR	2.1
1	D	257	ASP	2.1
1	G	460	ASP	2.1
1	I	281	ILE	2.1
1	L	85	GLY	2.1
1	K	130	THR	2.1
1	E	285	ALA	2.1
1	F	306	GLU	2.1
1	D	523	SER	2.1
1	I	466	SER	2.1
1	I	429	GLN	2.1
1	K	447	TYR	2.1
1	L	86	ALA	2.1
1	B	300	ILE	2.1
1	C	176	ILE	2.1
1	F	492	LEU	2.1
1	F	498	ASP	2.1
1	I	209	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	517	TYR	2.0
1	C	232	ALA	2.0
1	A	417	THR	2.0
1	G	444	LEU	2.0
1	D	248	LYS	2.0
1	L	304	PHE	2.0
1	B	466	SER	2.0
1	H	227	GLU	2.0
1	L	196	ASP	2.0
1	D	208	VAL	2.0
1	H	96	GLY	2.0
1	C	530	GLN	2.0
1	J	215	ASP	2.0
1	I	482	LEU	2.0
1	H	178	SER	2.0
1	C	510	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.